OPTIMAL MULTISTEP METHODS FOR SECOND ORDER INITIAL AND BOUNDARY VALUE PROBLEMS

by

RATNA BHATTACHARYA

DEPARTMENT OF MATHEMATICS

INDIAN INSTITUTE OF TECHNOLOGY KANPUR

February 1994

OPTIMAL MULTISTEP METHODS FOR SECOND ORDER INITIAL AND BOUNDARY VALUE PROBLEMS

A Thesis Submitted
in Partial Fulfilment of the Requirements
for the Degree of
DOCTOR OF PHILOSOPHY

By
RATNA BHATTACHARYA

to the
DEPARTMENT OF MATHEMATICS
**INDIAN INSTITUTE OF TECHNOLOGY
KANPUR**

FEBRUARY. 1994

Certificate

It is certified that the work contained in this thesis entitled "**Optimal Multistep Methods for Second Order Initial and Boundary Value Problems**", by **Ms. Ratna Bhattacharya**, has been carried out under my supervision and that this work has not been submitted elsewhere for a degree or diploma.

(R. K. S. Rathore)
Professor,
Department of mathematics,
Indian Institute of Technology,
Kanpur-208016, INDIA

February, 1994

To
My Parents

ACKNOWLEDGEMENTS

I wish to express my deep and sincere thanks to Professer R. K. S. Rathore for his guidance and encouragement throughout this thesis work. Thanks are due to Mrs.(Dr.) Rathore for her tolerance, during my long discussions with guide at their home.

I am thankful to my family members specially to my husband.

I would like to express my thanks to all faculty members and office staff in our department.

My thanks goes to my friends and colleagues, specially to Rangan, Joydip, Pratibha, Nisha, Snigdha, Subir, Amit.

Finally thanks goes to Mr. Metia for his careful printing.

February, 1994 Ratna Bhattacharya

CONTENTS

Page No.

INTRODUCTION 1

CHAPTER 1 : Optimal Multistep Methods for Special Second Order Differential Equations

1.1 : Introduction 12

1.2 : Optimal Multistep Methods for Second Order Differential Equations 15

1.3 : Optimal Multistep Methods Interpolatory for Polynomials 27

1.4 : Optimal Multistep Methods Interpolatory for Arbitrary Functions 37

CHAPTER 2 : Error Analysis of the Optimal Linear Multistep Methods for Initial Value Problem for Second Order Differential Equations

2.1 : Introduction 56

2.2 : Some Well Known Results for the Usual Method 58

2.3 : Optimal Multistep Methods for Initial Value Problems 62

2.4 : Relation between Optimal and Usual β-coefficients 64

2.5 : Convergence of β-Optimal Methods 67

2.6 : A Bound for the Discretization Error 70

2.7 : An A-Priori Bound for Round-off Error 72

2.8 : Linear Multistep Methods with Mildly Varying Coefficients 74

2.9 : A Bound for the Local Truncation Error 81

2.10: A Bound for the Discretization Error 84

2.11: Propagation of Round-off Error 86

2.12: Stability Analysis of Linear Multistep Methods with Varying Coefficients 87

CHAPTER 3 : Error Analysis of the Optimal Multistep Methods for Boundary Value Problems

3.1 : Introduction 103

3.2 : Some known Results on Linear Multistep Methods for Boundary Value Problems 106

3.3 : Relation Between Optimal and Usual β-coefficients 110

3.4 : Some Auxiliary Results 117

3.5 : Convergence Analysis 132

3.6 : Newton's Method for System of Nonlinear Equations 139

3.7 : Stability Analysis 156

CHAPTER 4 : Optimal Multistep Methods in $H^2(C_r)$-Space

4.1 : Introduction 184

4.2 : The Hilbert Space $H^2(C_r)$ 185

4.3 : Optimal Multistep Methods in $H^2(C_r)$-Space 191

4.4 : Optimal Multistep Methods in $H^2(C_r)$-Space Interpolatory for Polynomials 211

4.5 : Optimal Multistep Methods in $H^2(C_r)$-Space Interpolatory for a set of Preassigned Functions 220

4.6 : Behavior of the Coefficients As $r \longrightarrow \infty$ 231

4.7 : An Asymptotic Estimate of Local Truncation Error 237

CHAPTER 5 : Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space

5.1 : Introduction 256

5.2 : The Hilbert Space $L^2(\hat{C}_r)$ 257

5.3 : Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space 262

5.4 : Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space Interpolatory for Polynomials 283

5.5 : Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space Interpolatory for a Set of Preassigned Functions 289

5.6 : Behavior of the Coefficients as $r \longrightarrow \infty$ 299

CHAPTER 6 : Optimal Multistep Methods in $H^{(m)}_{a,b}$-Space

6.1 : Introduction 303

6.2 : Derivation of Kernel and the Representer of the Second Derivative Evaluation Functional 306

6.3 : Optimal Multistep Methods in $H^{(m)}_{a,b}$ Space 315

6.4 : Optimal Multistep Methods in $H^{(m)}_{a,b}$ Space Interpolatory for Polynomials 32

6.5 : Optimal Multistep Methods in $H^{(m)}_{a,b}$ Space Interpolatory for a set of Preassigned Functions 33

REFERENCES 34

INTRODUCTION

An initial value problem of the form

(1) $$y'' = f(x,y), \quad y(a) = A_0, \; y'(a) = B_0,$$

or a boundary value problem of the form

(2) $$y'' + f(x,y) = 0, \quad y(a) = A, \; y(b) = B,$$

in which f is a function of x and y and not of y′, and is continuous and Lipchitzian with respect to the second argument, occur frequently in various fields, e.g., in mechanical problems without dissipation and in astronomical problems. In the words of Henrici [96], "Indeed astronomers have for over a century used methods for integrating this kind of differential equations which are of the multistep type and which work without first derivatives."

A classical Linear k-step method of general form is given by

(3) $$\sum_{i=0}^{k} \alpha_i y_{n+k-i} + h^2 \sum_{i=0}^{k} \beta_i f_{n+k-i} = 0,$$

where $y_j = y(x_j)$, $f_j = f(x_j, y_j)$, $x_j = a + jh$, and h, α_j, β_j are constants, which do not depend on n. In such a formula, the coefficients are chosen in such a way that the associated linear difference operator given by

(4) $$L\,[y(x);h] \equiv \sum_{i=0}^{k} \alpha_i y(x+(n+k-i)h) + h^2 \sum_{i=0}^{k} \beta_i y''(x+(n+k-i)h),$$

is small for a solution of $y'' = f(x,y)$, that means, the method is made locally exact for polynomials of highest possible degree. The precision with respect to polynomial functions renders the

coefficients α_i's, β_i's independent of x_n. This property of coefficients is retained even when the formulae are made interpolatory for a maximal set of exponential functions $e^{\alpha x}$'s. However, if the formulae are made interpolatory with respect to a general class of functions, the coefficients α_i's, and β_i's would no more be independent of the point x_n under consideration.

To solve an initial value problems of the form (1), one can use linear multistep methods with constant coefficients. Indeed such methods are to be (i) Stormer's method (ii) Cowell's method , or some further special methods discussed by Collatz [53], Henrici [96], Jain [100], Lapidus and Seinfeld [125] and some others, provided with a special starting procedure. Many researchers have considered linear multistep methods for solving initial value problems and have discussed their convergence, consistency and stability criteria. Cash [31] has derived exponentially fitted multiderivative linear multistep methods of orders upto 5. He has considered the class of integration formulae, each containing a "built-in" local error estimate - a facility lacking in most other exponentially fitted formulae. Verwer [191], [192] has proposed a 3-rd order formula for the numerical integration of stiff systems of ordinary differential equations for first order initial value problems. This formula belongs to a special class of generalized linear multistep method formulae, of which the scalar coefficients are replaced by operator coefficients. Cooper [55] has considered a general linear multistep method for first order initial value problem and its order of convergence.

Theorems on linear multistep methods with constant stepsize

and constant formula were developed after the publication of Dahlquist's classical paper [58]. After 1969, linear multistep formulae have often been applied in practical codes as variable step size variable formula methods (VSVFM). Zlatev [195] has considered a general LMVSVFM of the form :

$$y_k = \sum_{i=1}^{s_k} \alpha_i(\bar{h}_k, s_k) y_{k-i} + \sum_{i=0}^{s_k} h_{k-i} \beta_i(\bar{h}_k, s_k) f(x_{k-i}, y_{k-i})$$

where $h_k = x_k - x_{k-1}$, $\bar{h}_k = (h_k, h_{k-1}, \ldots, h_{k-s_k})$, $s_k \le k$, $k = 1(1)N$. The coefficients α_i's and β_i's depend on the last s_k+1 and on the formula used at step k. He has defined a class of 3 ordinate LMVSVFM and has obtained some results concerning the zero-stability properties of these methods. Zlatev [199] has proved a formal definition of general LMVSVFM's and has shown some theorems concerning the consistency and the convergence of these methods. Marz Roswitha [132]-[134] has discussed various kinds of variable multistep methods and has shown several facts concerning stability, consistency and convergence of general two point boundary value problems of ordinary differential equations and has treated initial value problems as special cases.

Many authors have discussed stability criteria for linear multistep methods for ordinary differential equations. Dahlquist [59] in 1963, had defined A-stability for a linear multisetp method with constant coefficients, applied to a first order differential equation and had proved the well known result that the order of an A-stable linear multisetp method cannot exceed 2. Dahlquist [60] showed that a norm (Liapunov function) can be constructed for the stability and the error analysis of a linear multistep method for

the solution of a stiff non-linear system, provided that the system satisfies a monotonicity condition and the method possesses a property called G-stability. Dahlquist [62] has shown that G-stability and A-stability concepts are equivalent for multistep methods in their one leg formulation. Hairer and Turke [94] have shown to what extent this result also holds for Runge-Kutta methods. Veldhuizen [190] has proposed D-stability criterion for discretization methods for stiff, first order initial value problems. He has shown that D-stability is a necessary requirement for stability in the usual sense. Liniger [130] has given two easy-to-check conditions which, together, are sufficient and "almost necessary" for A-stability of linear multistep integration formulae. Most of the literature on stability of a numerical solution of ordinary differential equations is concerned with absolute stability, which tells whether the extraneous solutions introduced in the numerical solution grow or decay in magnitude. Because of difficulty in finding a high order absolutely stable numerical solution, researchers paid their attention to relative stability, which is a relation of the magnitude of the extraneous solutions to that of the true solution. Relative stability is mentioned by Hamming [95]. Ralston [153] has given a formal definition of relative stability of a numerical method for first order initial value problems and a simple computational scheme by which this definition can be tested. In order to solve initial value problems for systems of first order differential equations, where Jacobian of the right hand side of a linear multistep method has purely imaginary eigen values, the method is called stable

along the imaginary axis, according to Jeltsch [107] and Dekker [72]. Odeh and Liniger [145] have established nonlinear fixed -h stability similar to A-stability for implicit linear multistep formulae, when applied to nonlinear stable systems and have given sufficient criteria which guarantee the fixed -h stability of the global numerical error for various classes of non-linearities. Jeltsch [102], [105], [108], [109] and Bickart [24] have investigated some other stability criteria viz. A_0-stability, A(0)-stability, A[α]-stability and stiff stability for solving first order initial value problem. Many other authors viz., Chen [51], Cryer [57], Friedli and Jeltsch [85], Gear et. al.[88], [88], Grigorieff [93], Koloza [116], [117], Li Wangyaa [129], Nørsett [143], Oliveira and Patricio [147], Wanner et. al. [193]-[195], Widlund [196] have discussed linear multistep methods with constant coefficients for solving initial value problems and their various stability criteria.

Many researchers have used finite difference methods for solving two point boundary value problems. Asfar and Hussein [5], Tewarson et. al. [179], [181], [182] have considered high order numerical methods by writing the differential equation as a system of first order differential equations with general two point boundary conditions, with the help of the methodology of finite differences, splines and fundamental matrix. Many authors including Boutayeb and Twizell [25], Cash [32], Chawla [39]-[42], Tewarson [180], Twizell [184], Twizell and Boutayeb [185] have constructed high order finite difference schemes for solving two point boundary value problems with natural and mixed boundary conditions. Baboo

[7] and some other authors have considered finite difference methods for solving two point boundary value problems with periodic boundary conditions.

Much work has been done on finite difference methods for solving singular two point boundary value problems. Chawla and Katti [44]-[47] have considered a three point finite difference method for the singular two point boundary value problem of the from $y'' + (2/x)y' + f(x,y) = 0$, $y'(0) = 0$, $y(1) = a$ replacing y' and y'' by difference approximations. Chawla, Mckee and Shaw [48] have constructed a finite difference method based on uniform mesh for the problem $Lu = x^{\alpha}f(x,u)$, $u'(0) = 0$, $u(1) = A$, with $\alpha \geq 1$ and have shown $O(h^2)$ convergence of the method. Chawla [49] presents a new fourth order finite difference method for the weakly singular two point boundary value problem: $Lu = f(x,u)$, on $(u,1]$ subject to boundary condition $u(0) = A$, $u(1) = B$ for $0<\alpha<1$. The method reduces to the fourth order Numerov method for $u'' = f(x,u)$. Katti and Chopra [111] have studied the stability of modified Numerov method of Jain et. al. [101] for the class of singular two point boundary value problems of the from $y'' + (2/x)y' + f(x,y) = 0$, $y'(0) = 0$, $y(1) = a$. Balajan and Molokovic [9], Ciarlet [52], De Hoog and Weiss [69]-[71], Doedel and Reddien [76]-[78], Jain and Jain [101], and Pandey [149] and many others have worked on singular two point boundary value problems.

An ordinary differential equation can be solved by multistep methods based on quadrature formulae with precision for certain functions. Many researchers have shown that instead of using the usual quadrature formulae, optimal quadrature formulae with minimum

error norm corresponding to various classes of functions, are more effective. Sard [165], Davis [64], Barnhill [10]-[[13], [16]-[18], Barnhill and Wixom [15], Barnhill and Nelson [19], Barrer [20] and Larkin [126] have considered minimization of quadrature error in various manners with respect to weights to obtain the optimal quadrature formulae. Pinkus [150], Rabinowitz and Ritcher [151] and [152], Ritcher [157]-[159] have studied properties of such optimal formulae. Chawla and Kaul [36]-[38] and Kaul [113] have considered such optimal quadrature rules subject to interpolatory conditions for polynomials of degree less than or equal to the number of nodes. Kaul [112] and Finney and Price Jr. [82] have studied optimal quadrature rules with interpolatory conditions for arbitrary functions.

Some authors have studied linear multistep methods with varying coefficients and their convergence and stability criteria. Lambert [121], in 1970, has considered a linear multistep method with mildly varying coefficients of the form

$$\sum_{i=0}^{k} (\alpha_i + ha_j(x_n))\, y_{n+k-i} = h^2 \sum_{i=0}^{k} (\beta_i + hb_j(x_n))\, f_{n+k-i},$$

where $a_j(x_n)$ and $b_j(x_n)$ are functions specified by the particular differential equations under consideration, for solving a first order differential equation instead of using a constant method. He has shown that it is possible to control the weak stability characteristics of the method with varying coefficients. The weak instability associated with stable linear k-step usual method with order k+2 can be removed by using the linear multistep methods with varying coefficients, under some stabilizing conditions. We are

thus motivated to study a class of linear multistep methods with varying coefficients. Lambert and Sigurdsson [124] have shown that the application of a generalization of this stabilizing condition to a somewhat linear multistep method is applicable to systems of differential equations. Sanz-Serna [164] has proved some further results for the general class of Lambert-Sigurdsson method. Aguado and Correas [1], Aguado [2], Andreassen [3], Correas [54], Cronzeix and Lisbona [56], Marz [132]-[134], Varil'kov and Zagonov [189], Zlatev [197], [198], Sigurdsson [172] and some others have considered linear multistep methods with varying coefficients for solving differential equations of first order or systems of differential equations of first order.

Brij Bhusan [27] in 1986, has studied optimal multistep methods for solving first order differential equations. His thesis consists of a study of such methods which minimize the quadrature error or the local truncation error functional over a Hilbert space possessing a reproducing kernel function, in the numerical integration of a first order initial value problem. Such kind of multistep methods turn out to be multistep methods with varying coefficients.

No similar approach to get optimal fomulae in numerical solution of second order initial and two point boundary value problems, however, seems to have been taken up in the literature even though a need for this has been felt for quite some time (Gear [90]).

This thesis is an approach in this direction and consists of a study of the optimal multistep methods which minimize the norm of

local truncation error functional in the numerical integration of a second order initial value problem or a boundary value problem.

The body of this thesis consists of six chapters. The layout of each chapter is given below.

CHAPTER 1

This chapter is devoted to the derivation of various optimal multistep formulae in a general Hilbert space possessing a reproducing kernel function and the characterization of these formulae. The formulae with interpolatory constraints have been divided into two categories, one with interpolatory functions as polynomials of certain degree and the other with interpolatory functions being arbitrary.

It is shown that at each step, the coefficients of the optimal formulae give rise to a deterministic system of linear equations and that each formulae is characterized by it being locally interpolatory for a certain set of functions.

CHAPTER 2

This chapter deals with the convergence and the theoretical error analysis of optimal multistep formulae adopted for second order initial value problems. We first determine a relation between the β-coefficients of the β-optimal and the corresponding usual methods. The convergence of β-optimal method has been established next and an error bound for discretization error and an *a priori* bound for round off error of this method has been devised, the approach being delineated by Henrici. Then we study general linear multistep methods with varying coefficients for second order

initial value problems, the basic motivation coming from the work of Lambert on multistep methods with varying coefficients for first order initial value problems and the fact that our optimal methods are also of this category. We have established the convergence of such methods and derived the bounds for discretization error and propagation of round off errors. We have also given a stability analysis of linear multistep methods with varying coefficients.

CHAPTER 3

This chapter deals with some theoretical aspects of the β-optimal difference formulae corresponding to Cowell's usual formula with function evaluation at three points and Stormer's usual formula with function evaluation at one point, for solving two point boundary value problems of the form $y'' + f(x,y) = 0$, $y(a) = A$, $y(b) = B$, with $-\infty < \partial f/\partial y < \pi^2/(b-a)^2$. We establish the convergence of such an optimal difference method using the properties of monotone matrices and the convergence of Newton's method for systems of nonlinear optimal difference equations. Next, we establish stability theory for β-optimal and corresponding usual methods.

CHAPTERS 4,5 & 6

These chapters consist of numerical implementation of various optimal multistep formulae, derived in Chapter 1, adopted for second order initial and boundary value problems in three typical Hilbert spaces, viz. $H^2(C_r)$,$L^2(\hat{C}_r)$ and $H^{(m)}_{a,b}$ respectively. In $H^2(C_r)$ and $L^2(\hat{C}_r)$ spaces known reproducing Kernel functions have been used. The Kernel function for $H^{(m)}_{a,b}$ space has been derived.

Each of these chapters contains (i) the appropriate system of

linear equations, particularly simplified for the respective spaces, to determine the optimal coefficients; (ii) the locally interpolatory characterization of various optimal methods; and (iii) tabulated numerical results for various optimal methods for both initial and boundary value problems.

In case of optimal methods implemented for initial value problems, we use Cowell's three points and Stormers five points methods, and in case of optimal methods implemented for boundary value problems we use Stormers one point and Cowell's three points methods.

In chapters 4 and 5 we have also studied the limiting behaviour of the optimal β-coefficients as $r \longrightarrow \infty$. It has been shown that, the optimal β-coefficients have the limiting values equaling the β-coefficients of the corresponding usual method with maximal polynomial precision, with the same α-coefficients and the interpolatory constraints.

CHAPTER 1

OPTIMAL MULTISTEP METHODS FOR SPECIAL SECOND ORDER DIFFERENTIAL EQUATIONS

1.1 Introduction

Let us consider an initial value problem (IVP) with a special second order differential equation of the form

$$(1) \qquad y'' = f(x,y), \qquad y(a) = A_0, \; y'(a) = B_0,$$

where the function $f(x,y)$ satisfies the following conditions:

(i) $f(x,y)$ is defined and continuous in the strip $a \le x \le b$, $-\infty < y < \infty$, where a and b are finite.

(ii) There exists a constant L such that for any $x \in [a,b]$ and any two numbers y and y^*

$$|f(x,y) - f(x,y^*)| \le L\,|y - y^*|$$

For the numerical solution of the IVP (1) we introduce the points $x_n = a + nh$, $0 \le n \le N$, where $h = (b-a)N^{-1}$ and N is an appropriate integer. A linear multistep method with k steps, $k \ge 2$ of the form

$$(2) \qquad \sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0,$$

where $f_m = f(x_m, y_m)$ can be designed for the determination of the numbers y_n numerically which, it is hoped, approximate the values $y(x_n)$ of the true solution at the points x_n. We shall assume that $\alpha_0 \neq 0$, $|\alpha_k| + |\beta_k| > 0$. Here δ_{t0} is the Kronecker delta so that

the method (2) is an explicit method if $t = 0$, and is an implicit method if $t \neq 0$, say $t = 1$.

With the difference equation (2) for the differential equation (1), we associate the difference operator given by

$$(3) \qquad L[y(x);h] = \sum_{i=0}^{k} \alpha_i y(x+(k-i)h) - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i y''(x+(k-i)h).$$

The coefficients α_i's and β_i's are chosen in such a way that $L[y(x);h]$ is small for a solution of the given differential equation (1).

The present chapter is devoted to the derivation of various optimal formulae and their characterization. We shall develop optimal multistep methods of various forms which can be adopted for solving an initial value problem in such a way that the norm of the local truncation error functional of the corresponding method is pointwise minimum at each step over a Hilbert space H, possessing a reproducing kernel function.

Let D denote a point set contained in the space of a real orcomplex variable, and let H be a Hilbert space of functions $f(x)$, the domain of each $f \in H$ being D. If there exists a function $K(x,\bar{y})$ of two variables x, $y \in D$, which satisfies the inner product relation

$$(4) \qquad f(y) = (f(x), K(x,\bar{y})), \qquad f \in H, \; y \in D,$$

and also, for any fixed $y \in D$, $K(x,\bar{y}) \in H$, regarded as a function of x, then K is said to be a reproducing kernel function for H (Aronszain [4], Larkin [126]). Here the bar denotes complex conjugate.

A necessary and sufficient condition that H possesses a

reproducing kernel function is that, for every fixed $x \in D$, the linear functional $Lf = f(x)$ is bounded. That is, there exists a finite constant C_x, depending upon x, such that

$$(5) \qquad |f(x)| \leq C_x \|f\|, \quad \text{for all } f \in H.$$

This is a well known result due to Aronszain [4].

Furthermore, the reproducing kernel function for a Hilbert space, if it exists, is unique and satisfies the relation

$$(6) \qquad K(y,\bar{x}) \equiv \overline{K(x,\bar{y})}, \quad \text{for all } x,y \in D.$$

In this chapter, we shall assume that the k-th derivative evaluation functional $Dk_x : f \longrightarrow f^k(x)$, for $k = 2$, is a bounded linear functional in H for every $x \in D$. Further, we shall assume that H contains, as a subspace, the set of all polynomial functions.

In section 1.2, we obtain and characterize optimal multistep methods which are obtained by minimizing the local truncation error functional over a Hilbert space possessing a reproducing kernel function.

In section 1.3, we make a general multistep method exact for polynomials upto certain degree and find the corresponding optimal multistep method by minimizing the norm of local truncation error functional over a Hilbert space possessing a reproducing kernel function.

In section 1.4, interpolatory conditions are developed for a general set of preassigned functions subject to which the norm of local truncation error functional is minimized over a Hilbert space. The optimal methods obtained are shown to get characterized by interpolatory conditions for a certain set of functions.

In recent work, many researchers have considered boundary value problems (BVP) with a special second order differential equation of the form

(7) $$y'' + f(x,y) = 0, \qquad y(a) = A,\ y(b) = B,$$

where the function $f(x,y)$, in addition to satisfying the conditions (i) and (ii), have continuous partial derivatives with respect to y. Assume that

(8) $$u_* = \inf_{a \le x \le b} \frac{\partial f}{\partial y} \qquad \text{and} \qquad u^* = \sup_{a \le x \le b} \frac{\partial f}{\partial y},$$

then we shall study two categories of boundary value problems with either, $-\infty < u^* \le 0$, or, $0 < u^* < \pi^2/(b-a)^2$.

For solving a BVP of the form (7) one can use a multistep method of the form (2) with the associated difference operator of the form (3) in which f is to be replaced by -f. The optimal methods to be derived in this chapter remain applicable in solving such BVP's with the term f replaced by -f. However, for a BVP (7) it is not necessary to assume that $\alpha_0 \neq 0$ in (2).

In a multistep method (2), one or more α or β coefficients could be zero. Then we would like those α or β coefficients not to be present in the corresponding optimal methods.

1.2 Optimal Multistep Methods for 2-nd Order Differential Equations

Definition 1: Ignoring the round-off errors, let the numerical solution of the differential equation (1) satisfy

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0.$$

The true solution of the differential equation (1) satisfies

$$\sum_{i=0}^{k} \alpha_i y(x_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i y''(x_{n+k-i}) + T_n = 0,$$

where T_n is called the local truncation error at the n-th step (Jain [100]).

We shall assume that the 2-nd derivative evaluation functional is a bounded linear functional in H, with representer given by

$$(9) \qquad D2(t,\bar{x}_{n+k-i}) = \overline{\frac{\partial^2}{\partial z^2} K(z,\bar{t})} \Bigg|_{z=x_{n+k-i}} = \frac{\partial^2}{\partial z^2} K(t,\bar{z}) \Bigg|_{z=x_{n+k-i}} .$$

Now we shall establish the following result.

<u>Lemma 1:</u> Let $S = \{ K(t,\bar{x}_{n+k-i}), D2(t,\bar{x}_{n+k-i}) : i = 0\ (1)\ k\}$, for distinct points $x_n, x_{n+1}, \ldots, x_{n+k}$. Then S is a linearly independent set.

<u>Proof:</u> We know if x_{n+k-i}, $i = 0\ (1)\ k$ are k+1 distinct points, then the basic generalized Hermite interpolation polynomials $P_j(x)$, $Q_j(x)$, $R_j(x)$, $j = 0\ (1)\ k$, which are polynomials of degree 3k+2, satisfy

$P_j(x_{n+1-i}) = \delta_{ij}$, $\qquad Q_j(x_{n+1-i}) = 0$, $\qquad R_j(x_{n+1-i}) = 0$,

$P'_j(x_{n+1-i}) = 0$, $\qquad Q'_j(x_{n+1-i}) = \delta_{ij}$, $\qquad R'_j(x_{n+1-i}) = 0$,

$P''_j(x_{n+1-i}) = 0$, $\qquad Q''_j(x_{n+1-i}) = 0$, $\qquad R''_j(x_{n+1-i}) = \delta_{ij}$,

for $i = 0\ (1)\ k$, $j = 0\ (1)\ k$.

Now let

$$\sum_{i=0}^{k} c_i K(t,\bar{x}_{n+k-i}) + \sum_{i=0}^{k} d_i D2(t,\bar{x}_{n+k-i}) = 0.$$

Then taking inner product with $P_j(t)$ and $R_j(t)$, $j = 0(1)k$, we get

$$\sum_{i=0}^{k} c_i P_j(x_{n+k-i}) + \sum_{i=0}^{k} d_i P''_j(x_{n+k-i}) = 0, \quad j = 0\ (1)\ k,$$

which implies $c_j = 0$, $j = 0(1)k$, and

$$\sum_{i=0}^{k} c_i R_j(x_{n+k-i}) + \sum_{i=0}^{k} d_i R''_j\ (x_{n+k-i}) = 0, \quad j = 0\ (1)\ k,$$

which implies $d_j = 0$, $j = 0\ (1)\ k$. Hence the proof.

Now we shall find various optimal multistep methods.

Firstly, we shall find β-optimal method where optimization is done with respect to the β-coefficients while the α-coefficients are prefixed as in the usual method (2).

Let

$$(10) \qquad \sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} f_{n+k-i} = 0$$

be the β-optimal method corresponding to the usual method (2), where $\hat{\beta}_{i,n}$ are the optimal coefficients corresponding to the usual coefficients β_i, $i = \delta_{t0}(1)k$, at a point x_n, $0 \le n \le N-k$.

We consider the optimality criterion as the minimization of the norm of the local truncation error functional.

Now the local truncation error functional $\hat{T}_n$ at a point x_n of the optimal method (10) applied to a function $y(x)$, a true solution of the differential equation (1), is given by

$$\hat{T}_n y = \sum_{i=0}^{k} \alpha_i y(x_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} y''(x_{n+k-i}).$$

Therefore $\|\hat{T}_n\|$ at a point x_n in a Hilbert space (H) is given by

$$\|\hat{T}_n\|^2 = \| \sum_{i=0}^{k} \bar{\alpha}_i K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\hat{\beta}}_{i,n} D2(t,\bar{x}_{n+k-i}) \|^2,$$

where $D2(t,\bar{x}_{n+k-i})$ designates the representer for the 2-nd derivative evaluation functional at x_{n+k-i}, $i = 0(1)k$; $0 \le n \le N-k$.

Since $S = \{K(t,\bar{x}_{n+k-i}), D2(t,\bar{x}_{n+k-i})\colon i=0(1)k\}$, is linearly independent, to determine the optimal coefficients $\hat{\beta}_{i,n}$ we shall minimize $\|\hat{T}_n\|^2$ with respect to $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$, $0 \le n \le N-k$. According to Larkin [126], the first order change $\delta(\|\hat{T}_n\|^2)$, following a change $\delta(\hat{\beta}_{l,n})$, in $\hat{\beta}_{l,n}$, $l = \delta_{t0}(1)k$ is given by

$$\delta(\|\hat{T}_n\|^2) =$$

$$-h^2\left(\delta(\bar{\hat{\beta}}_{l,n}) D2(t,\bar{x}_{n+k-l}), \sum_{i=0}^{k}\bar{\alpha}_i K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\hat{\beta}}_{i,n} D2(t,\bar{x}_{n+k-i})\right)$$

$$-h^2\left(\sum_{j=0}^{k}\bar{\alpha}_j K(t,\bar{x}_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \bar{\hat{\beta}}_{j,n} D2(t,\bar{x}_{n+k-j}), \delta(\bar{\hat{\beta}}_{l,n}) D2(t,\bar{x}_{n+k-l})\right)$$

$$= -h^2\, \overline{\delta(\hat{\beta}_{l,n})}\left[\sum_{i=0}^{k}\alpha_i\left(D2(t,\bar{x}_{n+k-l}), K(t,\bar{x}_{n+k-i})\right)\right.$$

$$\left. - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n}\left(D2(t,\bar{x}_{n+k-l}), D2(t,\bar{x}_{n+k-i})\right)\right]$$

$$- \quad h^2\delta(\hat{\beta}_{l,n})\left[\sum_{j=0}^{k}\bar{\alpha}_j\left(K(t,\bar{x}_{n+k-j}), D2(t,\bar{x}_{n+k-l})\right)\right.$$

$$\left. - h^2 \sum_{j=\delta_{t0}}^{k} \bar{\hat{\beta}}_{j,n}\left(D2(t,\bar{x}_{n+k-j}), D2(t,\bar{x}_{n+k-l})\right)\right].$$

Now,

$$\left(D2(t,\bar{x}_{n+k-l}), K(t,\bar{x}_{n+k-i})\right) = \frac{\partial^2}{\partial z^2}\left(K(t,\bar{z}), K(t,\bar{x}_{n+k-i})\right)\Big|_{x=x_{n+k-l}}$$

$$= \frac{\partial^2}{\partial z^2} K(x_{n+k-1}, \bar{z}) \Big|_{z=x_{n+k-1}} = D2(x_{n+k-1}, \bar{x}_{n+k-1}).$$

Again,

$$\left(D2(t,\bar{x}_{n+k-1}), D2(t,\bar{x}_{n+k-1})\right) = \frac{\partial^2}{\partial z^2}\left(D2(t,\bar{x}_{n+k-1}), K(t,\bar{z})\right)\Big|_{z=x_{n+k-1}}$$

$$= \frac{\partial^2}{\partial z^2}\left(\frac{\partial^2}{\partial x^2} K(t,\bar{x})\Big|_{x=x_{n+k-1}}, K(t,\bar{z})\right)\Big|_{z=x_{n+k-1}}$$

$$= \frac{\partial^2}{\partial z^2}\left[\frac{\partial^2}{\partial x^2} K(z,\bar{x})\Big|_{x=x_{n+k-1}}\right]_{z=x_{n+k-1}}$$

$$= \frac{\partial^2}{\partial z^2} D2(z,\bar{x}_{n+k-1})\Big|_{z=x_{n+k-1}} = D2''(x_{n+k-1}, \bar{x}_{n+k-1}), \text{ say.}$$

Thus we get,

$$\delta(\| \hat{T}_n \|^2) =$$

$$- h^2 \overline{\delta(\hat{\beta}_{1,n})} \left[\sum_{1=0}^{k} \alpha_1 D2(x_{n+k-1}, \bar{x}_{n+k-1}) - h^2 \sum_{1=\delta_{t0}}^{k} \hat{\beta}_{1,n} D2''(x_{n+k-1}, \bar{x}_{n+k-1})\right]$$

$$- h^2 \delta(\hat{\beta}_{1,n}) \left[\sum_{j=0}^{k} \bar{\alpha}_j \overline{D2(x_{n+k-j}, \bar{x}_{n+k-1})} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} \overline{D2''(x_{n+k-j}, \bar{x}_{n+k-1})}\right].$$

Since, for minimizing $\hat{\beta}_{1,n}$, $\delta(\| \hat{T}_n \|^2)$ is to vanish for an arbitrary choice of $\delta(\hat{\beta}_{1,n})$, $1 = \delta_{t0}(1)k$; we have

$$(11) \qquad \sum_{1=0}^{k} \alpha_1 D2(x_{n+k-1}, \bar{x}_{n+k-1}) - h^2 \sum_{1=\delta_{t0}}^{k} \hat{\beta}_{1,n} D2''(x_{n+k-1}, \bar{x}_{n+k-1}) = 0.$$

This is the system of normal equations solving which we can obtain $\hat{\beta}_{1,n}$, $i = \delta_{t0}(1)k$, at a point x_n.

Comparing (10) and (11), we have the following theorem.

<u>Theorem 1:</u> The optimal method (10), where α_i, $i = 0(1)k$, are prefixed and the optimization is done with respect to $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$, is characterized by that it is locally interpolatory for the functions

$$\{D2(x,\bar{x}_{n+k-i}),\quad i = \delta_{t0}(1)k\}.$$

Now we shall find α-optimal multistep method, where optimization is done with respect to the α-coefficients, while the β-coefficients are prefixed as in the usual method (2). Let

$$\text{(12)}\qquad \sum_{i=0}^{k} \hat{\alpha}_{i,n}\, y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i\, f_{n+k-i} = 0$$

be the α-optimal method corresponding to the usual method (2), where $\hat{\alpha}_{i,n}$ are the optimal coefficients corresponding to the usual coefficients α_i, $i = 0(1)k$ at a point x_n, $0 \le n \le N-k$.

We consider the optimality criterion as the minimization of the norm of the local truncation error functional.

Now the local truncation error functional $\hat{T}_n^{\alpha}$ at a point x_n of the optimal method (12) applied to a function $y(x)$, a true solution of the differential equation (1), is given by

$$\hat{T}_n^{\alpha} y = \sum_{i=0}^{k} \hat{\alpha}_{i,n} y(x_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i y''(x_{n+k-i}).$$

As in Theorem 1, $\| \hat{T}_n^{\alpha} \|^2$ at a point x_n in a Hilbert space H possessing a reproducing kernel function is given by

$$\| \hat{T}_n^{\alpha} \|^2 = \| \sum_{i=0}^{k} \bar{\hat{\alpha}}_i K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\beta}_i D2(t,\bar{x}_{n+k-i} \|^2,$$

where $D2(t,\bar{x}_{n+k-i})$ designates the representer for the second

derivative evaluation functional at x_{n+k-i}, $i = 0(1)k$, $0 \le n \le N-k$, which is defined in (9).

Since, $S = \{K(t,\bar{x}_{n+k-i}),\ D2(t,\bar{x}_{n+k-i}):\ i=0(1)k\}$, is linearly independent, to determine the optimal coefficients $\hat{\alpha}_{i,n}$, we shall minimize $\| \hat{T}^{\alpha}_{n} \|^2$ with respect to $\hat{\alpha}_{i,n}$; $i = 0(1)k$, Proceeding as in Theorem 1, the first order change $\delta(\|\hat{T}^{\alpha}_{n}\|^2)$, following a change $\delta(\hat{\alpha}_{l,n})$, in $\hat{\alpha}_{l,n}$, $l = 0(1)k$ is given by

$$\delta(\| \hat{T}^{\alpha}_{n} \|^2) =$$

$$\left(\delta(\bar{\hat{\alpha}}_{l,n})K(t,\bar{x}_{n+k-l}), \sum_{i=0}^{k} \bar{\hat{\alpha}}_{i,n}K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\beta}_i D2(t,\bar{x}_{n+k-i})\right)$$

$$+ \left(\sum_{j=0}^{k} \bar{\hat{\alpha}}_{j,n}K(t,\bar{x}_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \bar{\beta}_j D2(t,\bar{x}_{n+k-j}), \delta(\bar{\hat{\alpha}}_{l,n})K(t,\bar{x}_{n+k-l})\right)$$

$$= \overline{\delta(\hat{\alpha}_{l,n})}\left[\sum_{i=0}^{k} \hat{\alpha}_{i,n}\left(K(t,\bar{x}_{n+k-i}),K(t,\bar{x}_{n+k-l})\right)\right.$$

$$\left.- h^2 \sum_{i=\delta_{t0}}^{k} \beta_i \left(K(t,\bar{x}_{n+k-l}),D2(t,\bar{x}_{n+k-i})\right)\right]$$

$$+ \delta(\hat{\alpha}_{l,n})\left[\sum_{j=0}^{k} \bar{\hat{\alpha}}_{j,n}\left(K(t,\bar{x}_{n+k-j}),K(t,\bar{x}_{n+k-l})\right)\right.$$

$$\left.- h^2 \sum_{j=\delta_{t0}}^{k} \bar{\beta}_j \left(D2(t,\bar{x}_{n+k-j}),K(t,\bar{x}_{n+k-l})\right)\right].$$

Since, $\left(D2(t,\bar{x}_{n+k-j}),K\ (t,\bar{x}_{n+k-l})\right) = D2(x_{n+k-l},\bar{x}_{n+k-j})$,

$$\delta(\| \hat{T}^{\alpha}_{n} \|^2)$$

$$= \overline{\delta(\hat{\alpha}_{l,n})}\left[\sum_{i=0}^{k} \hat{\alpha}_{i,n}\overline{K(x_{n+k-l},\bar{x}_{n+k-i})} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i \overline{D2(x_{n+k-l},\bar{x}_{n+k-i})}\right]$$

$$+ \delta(\hat{\alpha}_{l,n}) \left[\sum_{j=0}^{k} \bar{\hat{\alpha}}_{j,n} K(x_{n+k-l}, \bar{x}_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \bar{\beta}_j D2(x_{n+k-l}, \bar{x}_{n+k-j}) \right].$$

Since, for minimizing $\hat{\alpha}_{l,n}$, $\delta(\|\hat{T}_n^{\alpha}\|^2)$ is to vanish for an arbitrary choice of $\delta(\hat{\alpha}_{l,n})$, $l = 0(1)k$, we have

$$\sum_{j=0}^{k} \bar{\hat{\alpha}}_{j,n} K(x_{n+k-l}, \bar{x}_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \bar{\beta}_j D2(x_{n+k-l}, \bar{x}_{n+k-j}) = 0.$$

Taking complex conjugate on both sides, we get

$$\sum_{j=0}^{k} \hat{\alpha}_{j,n} K(x_{n+k-j}, \bar{x}_{n+k-l}) - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \overline{D2(x_{n+k-l}, \bar{x}_{n+k-j})} = 0,$$

or,

$$(13) \qquad \sum_{j=0}^{k} \hat{\alpha}_{j,n} K(x_{n+k-j}, \bar{x}_{n+k-l}) - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \frac{\partial^2}{\partial x^2} K(x, \bar{x}_{n+k-l}) \Big|_{x=x_{n+k-j}} = 0,$$

$$l = 0(1)k.$$

This is a system of normal equations, solving which we can obtain $\hat{\alpha}_{j,n}$, $j = 0(1)k$, at a point x_n.

Comparing (12) and (13), we get the following theorem.

<u>Theorem 2:</u> The optimal method (12) where β_i, $i = \delta_{t0}(1)k$, are prefixed and the optimization is done with respect to α_i's, $i=k(1)N-k$, is characterized by that it is locally interpolatory for the functions

$$\{K(x, \bar{x}_{n+k-l}), \quad l = 0(1)k\}.$$

Now we shall find the β-optimal methods under some restriction. Let

$$\sum_{l=0}^{k} \alpha_l y_{n+k-l} - h^2 \sum_{l=\delta_{t0}}^{k} \hat{\beta}_{l,n} f_{n+k-l} = 0$$

be the β-optimal method corresponding to the usual method (2). We

shall find the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$, at a point x_n, $0 \le n \le N-k$, subject to the condition that

$$\sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} = 1.$$

Note that, $\sum_{i=\delta_{t0}}^{k} \beta_{i,n} = 1$, is one of the consistency conditions for a usual method (2). For convenience, let us write

$$\hat{\beta}_{k,n} = 1 - \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n}.$$

Then the above β- optimal method becomes

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2\left(\hat{\beta}_{k,n} f_n + \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} f_{n+k-i}\right) = 0,$$

or,

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2\left(f_n - \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} f_n + \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} f_{n+k-i}\right) = 0,$$

or,

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} (f_{n+k-i} - f_n)\Big) = h^2 f_n. \tag{14}$$

The representer for the local truncation error functional for this method in a Hilbert space possessing a reproducing kernel function is given by

$$\hat{T}_n = \sum_{i=0}^{k} \bar{\alpha}_i K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k-1} \bar{\hat{\beta}}_{i,n}\left(D2(t,\bar{x}_{n+k-i}) - D2(t,\bar{x}_n)\right) - h^2 D2(t,\bar{x}_n).$$

To obtain the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$, the normal equations can be obtained by minimizing $\|\hat{T}_n\|^2$ with respect to $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$. Thus we obtain the normal equations

$$(h_l, \hat{T}_n) = 0, \quad l = \delta_{t0}(1)k-1,$$

with $h_l(t) = D2(t,\bar{x}_{n+k-l}) - D2(t,\bar{x}_n)$, which gives the following system of equations:

$$(15) \qquad \sum_{i=0}^{k} \alpha_i \left(D2(x_{n+k-i},\bar{x}_{n+k-l}) - D2(x_{n+k-i},\bar{x}_n) \right)$$

$$- \quad h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} \Big(D2''(x_{n+k-i},\bar{x}_{n+k-l}) \quad - \quad D2''(x_{n+k-i},\bar{x}_n)$$

$$- D2''(x_n,\bar{x}_{n+k-l}) + D2''(x_n,\bar{x}_n) \Big)$$

$$- h^2 \left(D2''(x_n,\bar{x}_{n+k-l}) - D2''(x_n,\bar{x}_n) \right) = 0, \quad l = \delta_{t0}(1)k-1.$$

This system of equations can be solved uniquely for $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$.

Thus we get the following theorem.

<u>Theorem 3:</u> The optimal multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} f_{n+k-i} = 0,$$

subject to the condition

$$\sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} = 1,$$

where α_i, $i = 0(1)k$, are prefixed and the optimization is done with respect to β_i's, $i = \delta_{t0}(1)k-1$, is characterized by that it is locally interpolatory for the functions

$$\{h_l(x): \ l = \delta_{t0}(1)k-1\}, \quad \text{where } h_l(x) = D2(x,\bar{x}_{n+k-l}) - D2(x,\bar{x}_n).$$

Now we shall find the α as well as β optimal method under some

restriction. Let

$$(16) \qquad \sum_{i=0}^{k} \hat{\alpha}_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} f_{n+k-i} = 0$$

be the α as well β optimal method corresponding to the usual method (2), subject to the condition

$$\sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} = 1.$$

We shall find the optimal coefficients $\hat{\alpha}_{i,n}$, $i = 0(1)k$, and $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$ at a point x_n, $0 \le n \le N-k$. For convenience, let

$$\hat{\beta}_{k,n} = 1 - \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n}.$$

Then as in (14), the optimal method (16) becomes

$$(17) \qquad \sum_{i=0}^{k} \hat{\alpha}_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} (f_{n+k-i} - f_n) \Big) = h^2 f_n.$$

The representer for the local truncation error functional for this method in a Hilbert space possessing an appropriate reproducing kernel function is given by

$$\hat{T}_n = \sum_{i=0}^{k} \bar{\hat{\alpha}}_{i,n} K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} \Big(D2(t,\bar{x}_{n+k-i}) - D2(t,\bar{x}_n) \Big) - h^2 D2(t,\bar{x}_n).$$

To obtain the optimal coefficients $\hat{\alpha}_{i,n}$, $i = 0(1)k$, as well as $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$, the normal equations can be obtained by minimizing $\|\hat{T}_n\|^2$ with respect to $\hat{\alpha}_{i,n}$, $i = 0(1)k$, and $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$. Thus we obtain the following normal equations

$(h_i, \hat{T}_n) = 0$, $i=\delta_{t0}(1)k-1$, where $h_i(x) = D2(x,\bar{x}_{n+k-i}) - D2(x,\bar{x}_n)$, and

$(g_l, \hat{T}_n) = 0, \ l = 0(1)k,$ where $g_l(x) = K(x, \bar{x}_{n+k-l})$.

Thus we get the following system of linear equations

$$(18) \qquad \sum_{i=0}^{k} \hat{\alpha}_{i,n} K(x_{n+k-i}, \bar{x}_{n+k-l})$$

$$-h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} \left(\overline{D2(x_{n+k-l}, \bar{x}_{n+k-i})} - \overline{D2(x_{n+k-l}, \bar{x}_n)} \right) - h^2 \overline{D2(x_{n+k-l}, \bar{x}_n)} = 0,$$

$l = 0(1)k$, and

$$(19) \qquad \sum_{i=0}^{k} \hat{\alpha}_{i,n} \left(D2(x_{n+k-i}, \bar{x}_{n+k-l}) - D2(x_{n+k-i}, \bar{x}_n) \right)$$

$$- \quad h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}_{i,n} \Big(D2''(x_{n+k-i}, \bar{x}_{n+k-l}) \quad - \quad D2''(x_{n+k-i}, \bar{x}_n)$$

$$- D2''(x_n, \bar{x}_{n+k-l}) + D2''(x_n, \bar{x}_n) \Big)$$

$$- h^2 \left(D2''(x_n, \bar{x}_{n+k-l}) - D2''(x_n, \bar{x}_n) \right) = 0, \quad l = \delta_{t0}(1)k-1.$$

The system of equations (18) and (19) can be solved uniquely for $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$ and $\hat{\alpha}_{i,n}$, $i = 0(1)k$.

Hence we get the following theorem.

<u>Theorem 4:</u> The optimal method

$$\sum_{i=0}^{k} \hat{\alpha}_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} f_{n+k-i} = 0,$$

where optimization is done with respect to $\hat{\alpha}_{i,n}$, $i = 0(1)k$; as well as $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$, subject to the condition

$$\sum_{i=\delta_{t0}}^{k} \hat{\beta}_{i,n} = 1,$$

is characterized by that it is locally interpolatory for the

functions, $\{h_l(x): l = \delta_{t0}(1)k-1\} \cup \{g_l(x): l = 0(1)k\}$, where

$$h_l(x) = D2(x,\bar{x}_{n+k-l})-D2(x,\bar{x}_n), \text{ and } g_l(x) = K(x,\bar{x}_{n+k-l}).$$

1.3 Optimal Multistep Methods Interpolatory for Polynomials

Definition 2: Let $F(x)$ be a function which we wish to approximate using the class of functions $\{g_n(x),\ n = 0,1,2...\}$. Let

$$F(x) \approx a_0g_0(x) + a_1g_1(x) + \dots\dots\dots + a_mg_m(x)$$

be an approximation of linear type to $F(x)$, where a_i, $i = 0(1)m$, are constants. We call an approximation exact or interpolatory, if the constants are chosen in such a way that on some fixed set of points $\{x_i, i=1(1)p\}$, the approximation and its first r_i derivatives, where r_i is a nonnegative integer, agree with $F(x)$ except for round-off (Ralston and Rabinowitz [154]).

Firstly, we shall find the β- optimal multistep methods interpolatory for polynomials upto degree q.

The usual multistep method

$$\sum_{l=0}^{k}\alpha_l y_{n+k-l} - h^2 \sum_{l=\delta_{t0}}^{k} \beta_l f_{n+k-l} = 0$$

can be written, using divided difference notation, as

$$\sum_{l=0}^{k}\alpha_l y_{n+k-l} - h^2 \sum_{l=\delta_{t0}}^{k} \gamma_l y''[x_{n+k-l}, x_{n+k-l+1}, \dots, x_{n+k-\delta_{t0}}] = 0.$$

If $q \le k+\delta_{t1}+1$, we can choose the coefficients $\{\gamma_i,\ i=\delta_{t0}(1)\ q+\delta_{t0}-2\}$ in such a manner that the method is exact for polynomials upto degree q. Thus we have

$$(20)\qquad \sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \gamma_i y''[x_{n+k-i},x_{n+k-i+1},..,x_{n+k-\delta_{t0}}]$$

$$= h^2 \sum_{i=q+\delta_{t0}-1}^{k} \gamma_i y''[x_{n+k-i},x_{n+k-i+1},..,x_{n+k-\delta_{t0}}],$$

in which optimization can be done with respect to the coefficients $\{\gamma_i,\ i=q+\delta_{t0}-1(1)k\}$. So we shall minimize the norm of the local truncation error functional with respect to these coefficients.

Now, if $D2(t,\bar{x})$ exists and is the representer for the 2-nd derivative evaluation functional in a Hilbert space H, then for any function $f(x) \in H$, $f''(x) = (f(t),D2(t,\bar{x}))$. The divided difference $y''[x_{n+k-i},x_{n+k-i+1},..,x_{n+k-\delta_{t0}}]$ being a linear combination of $y''(x_{n+k-i}),y''(x_{n+k-i+1}),..,y''(x_{n+k-\delta_{t0}})$, the representer, for $y''[x_{n+k-i},..,x_{n+k-\delta_{t0}}]$ in H, would be $D2[t;\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}]$, which is obtained as a divided difference of $D2(t,\bar{x})$ with respect to the 2-nd variable, which is a linear combination of $D2(t,\bar{x}_{n+k-i}),D2(t,\bar{x}_{n+k-i+1}),..,D2(t,\bar{x}_{n+k-\delta_{t0}})$. Then we have for any function $f(x) \in H$,

$$f''[x_{n+k-i},..,x_{n+k-\delta_{t0}}] = (f(t),D2[t;\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}])$$

The representer for the local truncation error functional $\hat{T}_n^q$ of the optimal method (20), in a Hilbert space possessing a reproducing kernel function is given by

$$\hat{T}_n^q = \sum_{i=0}^{k}\bar{\alpha}_i K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \bar{\gamma}_i D2[t,\bar{x}_{n+k-i},\bar{x}_{n+k-i+1},..,\bar{x}_{n+k-\delta_{t0}}]$$

$$- h^2 \sum_{i=q+\delta_{t0}-1}^{k} \bar{\hat{\gamma}}_i \; D2[t,\bar{x}_{n+k-i},\bar{x}_{n+k-i+1},..,\bar{x}_{n+k-\delta_{t0}}].$$

By Lemma 1, $S = \{K(t,\bar{x}_{n+k-i}), D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}]: \; i=0(1)k\}$ being linearly independent, its subset $S_1 = \{K(t,\bar{x}_{n+k-i}), i=0(1)k; D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}]: i=q+\delta_{t0}(1)k\}$ is linearly independent.

To minimize $\|\hat{T}^q_n\|^2$ with respect to $\hat{\gamma}_i$, $\delta(\|\hat{T}^q_n\|^2)$, following a change $\delta(\hat{\gamma}_i)$, in $\hat{\gamma}_i$, $i=q+\delta_{t0}-1\ (1)k$, is to vanish.

Proceeding as in the previous theorem, we get the following system of linear equations.

$$h^2 \sum_{i=q+\delta_{t0}-1}^{k} \hat{\gamma}_i (D2[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}], D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}])$$

$$= \sum_{i=0}^{k} \alpha_i (D2[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}], K(t,\bar{x}_{n+k-i}))$$

$$- h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \gamma_i (D2[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}], D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}]),$$

$$j = q+\delta_{t0}-1(1)k.$$

Thus we get a system of equations

$$(21) \qquad Px = Q,$$

where $P = (P_{ij})^{k}_{i,j=q+\delta_{t0}-1}$ is a matrix with

$$P_{ij} = (D2[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}], D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k-\delta_{t0}}])$$

$$= (D2''\,[x_{n+k-i},..,x_{n+k-\delta_{t0}}; \bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}]),$$

$$x = [\hat{\gamma}_{q+\delta_{t0}-1}, \hat{\gamma}_{q+\delta_{t0}}, \ldots\ldots\ldots, \hat{\gamma}_k]^T,$$

$$Q = [q_{q+\delta_{t0}-1}, q_{q+\delta_{t0}}, \ldots\ldots\ldots, q_k]^T \text{ with}$$

$$q_i = \frac{1}{h^2}\Big(\sum_{i=0}^{k}\alpha_i(D2[x_{n+k-i};\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}])$$

$$- h^2\sum_{i=\delta_{t0}}^{q+\delta_{t0}-2}\gamma_i(D2''[x_{n+k-i},..,x_{n+k-\delta_{t0}};\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}])\Big),$$

$$i = q+\delta_{t0}-1(1)k.$$

The matrix P can be obtained by performing elementary row and column operations on a leading submatrix of the matrix of the linear system (11). Therefore P must be nonsingular. So the system (21) can be solved uniquely, and the method (20) can be determined uniquely. By (20) and (21), we get the following theorem.

<u>Theorem 5:</u> The multistep method

$$\sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k}\beta_i f_{n+k-i} = 0$$

is interpolatory for polynomials of degree $q < k+\delta_{t1}+1$, and optimal with respect to β- coefficients if and only if it is interpolatory for the functions

$$\{x^i,\ i = 0(1)q\} \cup \{h_j(x),\ j=q+\delta_{t0}-1(1)k\},$$

where $h_j(x) = D2[x;\bar{x}_{n+k-j},..,\bar{x}_{n+k-\delta_{t0}}]$.

Now we shall find the α- optimal multistep methods which are interpolatory for polynomials upto degree q.

If m is the degree of the highest polynomial precision method corresponding to a multistep method of the form (2) with given β_i's, then the α-optimal methods can be made interpolatory for polynomials of degree q less than m.

The usual multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

can be written, using divided difference notation, as

$$\sum_{i=0}^{k} \gamma_i y[x_{n+k-i}, x_{n+k-i+1}, .., x_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0.$$

or,

$$(22) \qquad \sum_{i=0}^{q} \gamma_i y[x_{n+k-i}, x_{n+k-i+1}, .., x_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i}$$
$$= - h^2 \sum_{i=q+1}^{k} \gamma_i y\ [x_{n+k-i}, x_{n+k-i+1}, .., x_{n+k}].$$

If $q \le m-1$, we can choose the coefficients $\{\gamma_i,\ i = 0(1)q\}$ in such a manner that the method is exact for polynomials upto degree q. In such a method, optimization can be done with respect to the coefficients $\{\gamma_i,\ i=q+1(1)k\}$. So we shall minimize the norm of the local truncation error functional with respect to these coefficients.

Now the divided difference $y[x_{n+k-i}, x_{n+k-i+1}, .., x_{n+k}]$ being a linear combination of $y(x_{n+k-i})$, $y(x_{n+k-i+1}), \ldots\ldots, y(x_{n+k})$, its representer in H is $K[t;\bar{x}_{n+k-i}, \bar{x}_{n+k-i+1}, .., \bar{x}_{n+k}]$, which can be obtained as a divided difference of $K(t,\bar{x})$ with respect to its 2nd variable, which is a linear combination of $K(t,\bar{x}_{n+k-i}), .., K(t,\bar{x}_{n+k})$.

Then we have for any function $y(x) \in H$,

$$y[x_{n+k-i},..,x_{n+k}] = (y(t),K[t;\bar{x}_{n+k-i},..,\bar{x}_{n+k}]).$$

The representer for the local truncation error functional $\hat{T}_n^q$ of the optimal method, in a Hilbert space possessing a reproducing kernel function is given by

$$(23) \quad \sum_{i=0}^{q} \bar{\gamma}_i K[t,\bar{x}_{n+k-i},\bar{x}_{n+k-i+1},..,\bar{x}_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\beta}_i D2(t,\bar{x}_{n+k-i})$$

$$+ h^2 \sum_{i=q+1}^{k} \bar{\hat{\gamma}}_i K[t,\bar{x}_{n+k-i},\bar{x}_{n+k-i+1},..,\bar{x}_{n+k}].$$

By Lemma 1, $S_1 = \{K[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k}],D2(t,\bar{x}_{n+k-i}): i = 0(1)k\}$ is linearly independent. To minimize $\|\hat{T}_n^q\|^2$ with respect to $\hat{\gamma}_i$, $\delta(\|\hat{T}_n^q\|^2)$, following a change $\delta(\hat{\gamma}_i)$, in $\hat{\gamma}_i$, $i = q+1\ (1)\ k$, is to vanish. Proceeding as in Theorem 5, we get the following system of linear equations

$$- \sum_{i=q+1}^{k} \hat{\gamma}_i (K[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k}],K[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k}])$$

$$= \sum_{i=0}^{q} \gamma_i (K[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k}],K[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k}])$$

$$- h^2 \sum_{i=\delta_{t0}}^{k} \beta_i (D2(t,\bar{x}_{n+k-i}),K[t,\bar{x}_{n+k-j},..,\bar{x}_{n+k}]), \quad j=q+1(1)k.$$

which may be rewritten as

$$(24) \qquad \tilde{P}\,\tilde{x} = \tilde{Q},$$

where $\tilde{P} = (\tilde{P}_{ij})_{i,j=q+1}^{k}$ is a matrix with

$$\tilde{P}_{ij} = K[x_{n+k-j},..,x_{n+k};\bar{x}_{n+k-i},..,\bar{x}_{n+k}],$$

$$\tilde{X} = [\hat{\gamma}_{q+1}, \hat{\gamma}_{q+2},........,\hat{\gamma}_k]^T,$$

$$\tilde{Q} = [\tilde{q}_{q+1},\tilde{q}_{q+2},........,\tilde{q}_k]^T \text{ with}$$

$$\tilde{q}_i = - \sum_{i=0}^{q} \gamma_i K[x_{n+k-j},..,x_{n+k};\bar{x}_{n+k-i},..,\bar{x}_{n+k}]$$

$$+ h^2 \sum_{i=\delta_{t0}}^{k} \beta_i D2(x_{n+k-j},..,x_{n+k} ; \bar{x}_{n+k-i}), \ j=q+1(1)k,$$

where $D2(x_{n+k-j},..,x_{n+k};\bar{x}_{n+k-i})$ is the divided difference of $D2(t,\bar{z})$ with respect to its first variable. The matrix $\tilde{P}$ can be obtained by performing elementary row and column operations on a leading submatrix of the matrix of the linear system (13). Therefore $\tilde{P}$ must be nonsingular. So the system (24) can be solved uniquely, and the method (23) can be determined uniquely. By (23) and (24), we get the following theorem.

<u>Theorem 6:</u> The multistep method

$$\sum_{i=0}^{k} \hat{\alpha}_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

is interpolatory for polynomials of degree $q \le m-1$, and optimal with respect to α- coefficients if and only if it is interpolatory for the functions

$$\{x^i, \ i = 0(1)q\} \cup \{h_j(x), \ j = q+1(1)k\},$$

where $h_j(x) = K[x_{n+k-j},..,x_{n+k};\bar{x}]$.

Now we shall find the α as well as β-optimal multistep methods which is interpolatory for polynomials upto degree q.

The usual multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

can be written, using divided difference notation, as

$$\sum_{i=0}^{k} \lambda_i \; y[x_{n+k-i},\ldots,x_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{k} \mu_i y'' \; [x_{n+k-i},\ldots,x_{n+k}] = 0.$$

We can choose the coefficients $\{\lambda_i,\ i=0(1)q\}$ and $\{\mu_i,\ i=\delta_{t0}(1)\ q+\delta_{t0}-2\}$ in such a manner that the method is exact for polynomials upto degree q. Thus we have

$$\sum_{i=0}^{q} \lambda_i \; y[x_{n+k-i},\ldots,x_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \mu_i y'' \; [x_{n+k-i},\ldots,x_{n+k}]$$

$$=-\sum_{i=q+1}^{k} \lambda_i \; y[x_{n+k-i},\ldots,x_{n+k}] + h^2 \sum_{i=q+\delta_{t0}-1}^{k} \mu_i y'' \; [x_{n+k-i},\ldots,x_{n+k}],$$

in which optimization can be done with respect to the coefficients $\{\lambda_i,\ i = q+1(1)k\}$ and $\{\mu_i,\ i = q+\delta_{t0}-2(1)k\}$. So we shall minimize the norm of the local truncation error functional with respect to these coefficients. The representer for the local truncation error functional $\hat{T}_n^q$ of the optimal method, in a Hilbert space possessing a reproducing kernel function is given by

$$\sum_{i=0}^{q} \bar{\lambda}_i \; K[t;\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}] - h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \bar{\mu}_i D2[t;\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}]$$

$$= - \sum_{i=q+1}^{k} \bar{\hat{\lambda}}_i \; K[t;\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}] + h^2 \sum_{i=q+\delta_{t0}-1}^{k} \bar{\hat{\mu}}_i D2[t;\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}]$$

By Lemma 1, $S_1=\{K[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k}],D2[t,\bar{x}_{n+k-i},..,\bar{x}_{n+k}]: \quad i=0(1)k\}$ is linearly independent. To minimize $\|\hat{T}_n^q\|^2$ with respect to $\hat{\lambda}_i$ and $\hat{\mu}_i$, $\delta(\|\hat{T}_n^q\|^2)$ following a change $\delta(\hat{\lambda}_i)$ in $\hat{\lambda}_i$, $i=q+1(1)k$, and $\delta(\|\hat{T}_n^q\|^2)$, following a change $\delta(\hat{\mu}_i)$, in $\hat{\mu}_i$, $i=q+\delta_{t0}-1(1)k$ are to vanish. Proceeding as in Theorem 5, we get the normal equations,

$$(25) \qquad - \sum_{i=q+1}^{k} \hat{\lambda}_i K[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}]$$

$$+ h^2 \sum_{i=q+\delta_{t0}-1}^{k} \hat{\mu}_i D2[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}]$$

$$= \sum_{i=0}^{q} \lambda_i K[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}]$$

$$- \qquad h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \mu_i D2[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}],$$

$$l = q+1(1)k,$$

and

$$(26) \qquad - \sum_{i=q+1}^{k} \hat{\lambda}_i D2[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}]$$

$$+ h^2 \sum_{i=q+\delta_{t0}-1}^{k} \hat{\mu}_i D2'' \; [x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}]$$

$$= \sum_{i=0}^{q} \lambda_i D2[x_{n+k-1},\ldots,x_{n+k};\bar{x}_{n+k-1},\ldots,\bar{x}_{n+k}]$$

$$- h^2 \sum_{i=\delta_{t0}}^{q+\delta_{t0}-2} \mu_i D2'' [x_{n+k-i},\ldots,x_{n+k};\bar{x}_{n+k-l},\ldots,\bar{x}_{n+k}],$$

$$l = q+\delta_{t0}-1(1)k.$$

Thus we get a system of linear equations, written in matrix form as

$$\begin{bmatrix} A & B \\ -B^* & C \end{bmatrix} \begin{bmatrix} \lambda \\ \mu \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \end{bmatrix}, \tag{27}$$

where

$$A = (A_{ij})_{\substack{i=q+1(1)k, \\ j=q+1(1)k}} \qquad A_{ij} = -K[x_{n+k-i},\ldots,x_{n+k};\bar{x}_{n+k-j},\ldots,\bar{x}_{n+k}],$$

$$B = (B_{ij})_{\substack{i=q+1(1)k \\ j=q+\delta_{t0}-1(1)k}}, \qquad B_{ij} = D2[x_{n+k-i},\ldots,x_{n+k};\bar{x}_{n+k-j},\ldots,\bar{x}_{n+k}],$$

$$C = (C_{ij})_{\substack{i=q+\delta_{t0}-1(1)k, \\ j=q+\delta_{t0}-1(1)k}} \qquad C_{ij} = D2''[x_{n+k-j},\ldots,x_{n+k};\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}],$$

$$\lambda = \left(\hat{\lambda}_{q+1},\hat{\lambda}_{q+2},\ldots,\hat{\lambda}_k\right)^T, \quad \mu = \left(\hat{\mu}_{q+\delta_{t0}-1},\hat{\mu}_{q+\delta_{t0}},\ldots,\hat{\mu}_k\right)^T,$$

$d_1 = (d_{1,q+1},d_{1,q+2},\ldots,d_{1,k})^T$, with

$$d_{1,i} = \sum_{j=0}^{q} \lambda_j K[x_{n+k-i},\ldots,x_{n+k};\bar{x}_{n+k-j},\ldots,\bar{x}_{n+k}]$$

$$- h^2 \sum_{j=\delta_{t0}}^{q+\delta_{t0}-2} \mu_i D2[x_{n+k-i},\ldots,x_{n+k};\bar{x}_{n+k-j},\ldots,\bar{x}_{n+k}], \quad l=q+1(1)k,$$

$d_2 = (d_{2,q+\delta_{t0}-1},d_{2,q+\delta_{t0}},\ldots,d_{2,k})^T$, with

$$d_{2i} = \sum_{j=0}^{q} \lambda_j D2[x_{n+k-j},\ldots,x_{n+k};\bar{x}_{n+k-i},\ldots,\bar{x}_{n+k}]$$

$$- h^2 \sum_{j=\delta_{to}}^{q+\delta_{to}-2} \mu_j D2'' \, [x_{n+k-j}, \ldots, x_{n+k}; \bar{x}_{n+k-i}, \ldots, \bar{x}_{n+k}], \quad i=q+\delta_{to}-1(1)k.$$

Thus we get the following theorem.

<u>Theorem 7:</u> The multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{to}}^{k} \beta_i f_{n+k-i} = 0$$

is interpolatory for polynomials of degree q, and optimal with respect to α as well as β coefficients if and only if it is interpolatory for the functions

$$\{x^i, \ i=0(1)q\} \cup \{h_j(x), \ j=q+1(1)k\} \cup \{g_j(x), \ j=q+\delta_{to}-1(1)k\}$$

where $h_j(x) = K \, [x_{n+k-j}, \ldots, x_{n+k}; \bar{x}]$

and $g_j(x) = D2[x; \bar{x}_{n+k-j}, \ldots, \bar{x}_{n+k-\delta_{to}}]$.

1.4 <u>Optimal Multistep Methods Interpolatory for Arbitrary Functions</u>

We shall find the optimal multistep methods interpolatory for arbitrary functions with the help of Lagrangian multipliers.

<u>Lemma 2</u> : A necessary and sufficient condition that the multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{to}}^{k} \beta_i f_{n+k-i} = 0$$

be interpolatory for functions $f_1, f_2, \ldots, f_q$ is that for every function $\phi \in \text{span}\,\{f_1, f_2, \ldots, f_q\}$ for which

$$\phi\ (x_{n+k-i}) = 0, \quad i = 0(1)k,$$

there holds

$$\sum_{i=\delta_{t0}}^{k} \beta_i \phi''(x_{n+k-i}) = 0.$$

Proof : The necessity part is obvious. For sufficiency assume that the stated conditions hold. Consider the system

$$(28) \qquad \sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j}) = h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_i''(x_{n+k-j}), \quad 1 \le i \le q$$

of linear equations in α_j, $j = 0(1)k$. Applying elementary row operations on the system (28), we can reduce it to one in which the matrix is in a row reduced echolon form. In this system the existence of a nonzero augmented entry corresponding to a zero row of the matrix would contradict the stated conditions. Hence, the system (28) is consistent, completing the proof of the lemma.

In view of the above lemma and its proof, we can say that if a multistep method is interpolatory for span $\{f_1,f_2,\ldots,f_q\}$ then there exists $q_1 \le k+1$ functions g_1, $g_2,\ldots,g_{q_1}$ in the span $\{f_1,f_2,\ldots.,f_q\}$ such that

$$\text{rank}\ [g_i(x_{n+k-j})]_{\substack{i=1(1)q_1 \\ j=0(1)k}} = q_1,$$

and the multistep method is interpolatory for span $\{f_1,f_2,\ldots,f_q\}$ if and only if, it is interpolatory for g_1, $g_2,\ldots,g_{q_1}$. Hence with preprocessing, if necessary, we can assume that f_1, $f_2,\ldots,f_q$ themselves are such that

(29) $$\operatorname{rank}\,[f_i(x_{n+k-j})]_{\substack{i=1(1)q\\ j=0(1)k}} = q \le k+1.$$

If $q = k+1$, all the coefficients α_i's get uniquely determined and no optimization of error will be possible. Hence for α-optimal interpolatory method, we will assume that $q < k+1$.

<u>Lemma 3</u> : A necessary and a sufficient condition that the multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

be interpolatory for arbitrary functions $f_1, f_2, \ldots, f_q$ is that for every function $\phi \in \operatorname{span}\{f_1, f_2, \ldots, f_q\}$ for which

$$\phi''(x_{n+k-i}) = 0, \quad i = \delta_{t0}(1)k,$$

there holds

$$\sum_{i=0}^{k} \alpha_i \phi(x_{n+k-i}) = 0.$$

<u>Proof</u> : Proof follows similar to the proof of Lemma 2.

With the similar lines of arguments, we see that if a multistep method is interpolatory for span $\{f_1, f_2, \ldots, f_q\}$, then there exists q_1 $(\le k+\delta_{t1})$ functions $g_1, g_2, \ldots, g_{q_1}$ in the span $\{f_1, f_2, \ldots, f_q\}$ such that

$$\operatorname{rank}\,[g_i''(x_{n+k-j})]_{\substack{i=1(1)q_1\\ j=\delta_{t0}(1)k}} = q_1,$$

and the multistep method is interpolatory for span $\{f_1, f_2, \ldots, f_q\}$ if and only if, it is interpolatory for $g_1, g_2, \ldots, g_{q_1}$. Hence we can assume that $f_1, f_2, \ldots, f_q$ themselves are such that

(30) $$\operatorname{rank}\left[f_i''(x_{n+k-j})\right]_{\substack{i=1(1)q\\ j=\delta_{t0}(1)k}} = q \le k+\delta_{t1}.$$

If $q = k+\delta_{t1}$, all the coefficients β_i's get uniquely determined and no optimization of error will be possible. Hence for β-optimal interpolatory method, we will assume that $q < k+\delta_{t1}$.

<u>Lemma 4</u> : A necessary and sufficient condition that the multistep method

$$\sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k-1}\beta_i(f_{n+k-i}-f_n) - h^2 f_n = 0$$

be interpolatory for linearly independent arbitrary functions f_1, $f_2,\ldots,f_q$ is that for every function $\phi \in \operatorname{span}\{f_1,f_2,\ldots,f_q\}$ for which

$$\phi''(x_{n+k-i}) - \phi''(x_n) = 0, \quad i = \delta_{t0}(1)k-1,$$

there holds

$$\sum_{i=0}^{k}\alpha_i\phi(x_{n+k-i}) - h^2\phi''(x_n) = 0.$$

<u>Proof</u> : The necessity part is obvious. For sufficiency, assume that the stated conditions hold. Consider the system

(31) $$h^2\sum_{j=\delta_{t0}}^{k-1}\beta_j\Big(f_i''(x_{n+k-j})-f_i''(x_n)\Big) = \sum_{j=0}^{k}\alpha_j f_i(x_{n+k-j})-h^2 f_i''(x_n),$$

$$1 \le i \le q,$$

of linear equations in β_j, $j = \delta_{t0}(1)k-1$. With the similar arguments given in Lemma 2, the sufficiency part follows.

Thus, we can say that if a multistep method is interpolatory

for span $\{f_1, f_2, \ldots, f_q\}$, then there exists $q_1 \le k-1+\delta_{t1}$ functions functions $g_1, g_2, \ldots, g_{q_1}$ in the span$\{f_1, f_2, \ldots, f_q\}$, such that

$$\operatorname{rank}\left(g_i''(x_{n+k-j}) - g_i''(x_n)\right)_{\substack{i=1(1)q_1 \\ j=\delta_{t0}(1)k-1}} = q_1,$$

and the multistep method is interpolatory for span $\{f_1, f_2, \ldots, f_q\}$ if and only if, it is interpolatory for $g_1, g_2, \ldots, g_{q_1}$. So, we can assume that $f_1, f_2, \ldots, f_q$ themselves are such that

(32) $$\operatorname{rank}\left(f_i''(x_{n+k-j}) - f_i''(x_n)\right)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-1}} = q \le k-1+\delta_{t1}.$$

If $q = k-1+\delta_{t1}$, all the coefficients β_i's get uniquely determined and no optimization of error will be possible. Hence for optimal interpolatory method with restriction we will assume that $q < k-1+\delta_{t1}$.

First, we shall find β-optimal multistep method interpolatory for a set of arbitrary functions. Let

(33) $$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n} f_{n+k-i} = 0$$

be the β-optimal method interpolatory for functions $f_1, f_2, \ldots, f_q$. The representer for the local truncation error functional in a Hilbert space possessing a reproducing kernel function is given by

$$\hat{T}^F_n = \sum_{i=0}^{k} \bar{\alpha}_i K(t, \bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\hat{\beta}}^F_{i,n} D2(t, \bar{x}_{n+k-i}).$$

To obtain the optimal coefficients $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$, we have to minimize, $\|\hat{T}^F_n\|^2$ subject to the condition, $(\hat{T}^F_n, f_m) = 0$, $m = 1(1)q$. Using the method of Lagrange multipliers, we get the following

system of linear equations to determine $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$.

$$\begin{bmatrix} A & -F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix}, \tag{34}$$

where

$$A = (A_{ij})_{\substack{i=\delta_{t0}(1)k \\ j=\delta_{t0}(1)k}}, \quad \text{with} \quad A_{ij} = D2''(x_{n+k-j}, \bar{x}_{n+k-i}),$$

$$F = (F_{ij})_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k}}, \quad \text{with} \quad F_{ij} = f_i''(x_{n+k-j}),$$

$$b = h^2\left(\hat{\beta}^F_{\delta_{t0},n}, \hat{\beta}^F_{\delta_{t0}+1,n}, \ldots, \hat{\beta}^F_{k,n}\right)^T, \qquad \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q)^T,$$

$$c = \left(c_{\delta_{t0}}, c_{\delta_{t0}+1}, \ldots, c_k\right)^T, \quad \text{with } c_i = \sum_{j=0}^{k} \alpha_j D2(x_{n+k-j}, \bar{x}_{n+k-i}),$$

and

$$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T, \qquad \text{with } \tilde{f}_i = \sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j}).$$

Assuming the functions f_m, $m = 1(1)q$, to be such that the above matrix is invertible, it follows that the unique solution $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$, thus obtained will satisfy the required optimal interpolatory condition.

Now we shall characterize the β-optimal multistep method interpolatory for a set of functions. For simplicity in the form of characterization, we assume that the last p columns in the matrix (30) are linearly independent. In general, our assumption is that some p columns of the matrix (30) are linearly independent. Then in the corresponding characterization, the indices of these columns instead of the last p columns in the simpler case would appear in the formulation.

Let the interpolatory condition appearing in (34),

$$Fb = f$$

be rewritten as

$$[E \mid P]\begin{bmatrix} d \\ e \end{bmatrix} = f,$$

where

(35) $$E = \left(f_i''\ (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-q}}, \quad P = \left(f_i''\ (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=k-q+1(1)k}},$$

(36) $$d = \left(\hat{\beta}^F_{\delta_{t0},n}, \ldots, \hat{\beta}^F_{k-q,n}\right)^T, \quad e = \left(\hat{\beta}^F_{k-q+1,n}, \ldots, \hat{\beta}^F_{k,n}\right)^T,$$

(37) $$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T, \qquad \text{with } \tilde{f}_i = \frac{1}{h^2} \sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j}).$$

Then, $e = P^{-1}(f - Ed)$. Let

(38) $$r = P^{-1}f = (r_1, r_2, \ldots, r_q)^T, \quad G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}},$$

then $e = r - Gd$, and the method (33) can be written as

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-q} \hat{\beta}^F_{i,n} f_{n+k-i} - h^2 \sum_{i=k-q+1}^{k} \hat{\beta}^F_{i,n} f_{n+k-i} = 0,$$

or,

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-q} \hat{\beta}^F_{i,n} f_{n+k-i}$$

$$- h^2 \sum_{i=k-q+1}^{k} \left(r_{i+q-k} - \sum_{j=\delta_{t0}}^{k-q} \hat{\beta}^F_{j,n} g_{i+q-k,\, j+1-\delta_{t0}}\right) f_{n+k-i} = 0,$$

which is the same as

(39) $$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=k-q+1}^{k} r_{i+q-k} f_{n+k-i} -$$

$$- h^2 \sum_{i=\delta_{t0}}^{k-q} \hat{\beta}^F_{i,n} \left(f_{n+k-i} - \sum_{j=k-q+1}^{k} g_{j+q-k,\, i+1-\delta_{t0}} f_{n+k-j} \right) = 0.$$

Hence we get the following Theorem:

Theorem 8: An optimal multistep method

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n} f_{n+k-i} = 0$$

with prefixed α_i's, is interpolatory for functions $f_1, f_2, \ldots, f_q$ satisfying (30), if and only if it is interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i \; : \; i = \delta_{t0}(1)k-q\},$$

where $h_i = D2(x, \bar{x}_{n+k-i}) - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1-\delta_{t0}} D2(x, \bar{x}_{n+k-j})$

where g_{ij}'s are defined in (38) and (35).

Proof: From equation (39), we see that to determine the optimal coefficients $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k-q$, the normal equations can be obtained by minimizing the norm of local truncation error functional $\hat{T}^F_n$ for the method (39) with respect to the coefficients $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k-q$. Thus we get the system of normal equations

$$(h_i \, , \, \hat{T}^F_n) = 0, \quad i = \delta_{t0}(1)k-q,$$

where $h_i = D2(x, \bar{x}_{n+k-i}) - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1-\delta_{t0}} D2(x, \bar{x}_{n+k-j})$ and the method (39) is also interpolatory for the functions $f_1, f_2, \ldots, f_q$.

Hence the proof.

Now we shall find an α-optimal method interpolatory for linearly independent arbitrary functions.

Let

$$(40) \qquad \sum_{i=0}^{k} \hat{\alpha}^{F}_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

be an α-optimal method interpolatory for arbitrary functions f_1, $f_2, \ldots\ldots, f_q$. The representer for the local truncation error functional in a Hilbert space possessing a reproducing kernel function is given by

$$\hat{T}^{F}_{n} = \sum_{i=0}^{k} \bar{\hat{\alpha}}^{F}_{i,n} K(t, \bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k} \bar{\beta}_i D2(t, \bar{x}_{n+k-i})$$

To obtain the optimal coefficients $\hat{\alpha}^{F}_{i,n}$, $i = 0(1)k$, we have to minimize, $\|\hat{T}^{F}_{n}\|^2$ subject to the condition $(\hat{T}^{F}_{n}, f_m) = 0$, $m = 1(1)q$. Using method of Lagrange multipliers, we get the following system of linear equations to determine $\hat{\alpha}^{F}_{i,n}$, $i = 0(1)k$.

$$(41) \qquad \begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} a \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where F^* is the conjugate transpose of F.

$A = (A_{ij})_{\substack{i=0(1)k \\ j=0(1)k}}$, with $A_{ij} = K(x_{n+k-j}, \bar{x}_{n+k-i})$,

$F = (F_{ij})_{\substack{i=1(1)q \\ j=0(1)k}}$, with $F_{ij} = f_i(x_{n+k-j})$,

$a = \left(\hat{\alpha}^{F}_{0,n}, \hat{\alpha}^{F}_{1,n}, \ldots\ldots, \hat{\alpha}^{F}_{k,n}\right)^T$, $\lambda = (\lambda_1, \lambda_2, \ldots\ldots, \lambda_q)^T$,

$$c = (c_0, c_1, \ldots, c_k)^T, \quad \text{with } c_i = h^2 \sum_{j=\delta_{t0}}^{k} \beta_j D2(x_{n+k-i}, \bar{x}_{n+k-j}),$$

and

$$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T, \quad \text{with } \tilde{f}_i = h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_i'' (x_{n+k-j}).$$

Assuming the functions $\tilde{f}_m$'s to be such that the above matrix i invertible, $\hat{\alpha}^F_{i,n}$, $i = 0(1)k$, can be determined uniquely.

Now we shall characterize the α-optimal multistep method interpolatory for a given set of functions. For simplicity in the form of characterization, we assume that the last p columns in the matrix (29) are linearly independent. In general, our assumption is that some p columns of the matrix (29) are linearly independent. Then in the corresponding characterization, the indices of these columns instead of the last p columns in the simpler case would appear in the formulation.

Let the interpolatory condition appearing in (41),

$$Fa = f$$

be rewritten as

$$[E \mid P] \begin{bmatrix} d \\ e \end{bmatrix} = f,$$

where

(42) $$E = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=0(1)k-q}}, \quad P = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=k-q+1(1)k}},$$

(43) $$d = \Big(\hat{\alpha}^F_{0,n}, \ldots, \hat{\alpha}^F_{k-p,n}\Big)^T, \quad e = \Big(\hat{\alpha}^F_{k-p+1,n}, \ldots, \hat{\alpha}^F_{k,n}\Big)^T$$

(44) $\quad f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T, \quad$ with $\tilde{f}_i = h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_i'' (x_{n+k-j})$.

Then, $\quad e = P^{-1}(f - Ed)$. Let

(45) $\quad r = P^{-1} f = (r_1, r_2, \ldots, r_q)^T, \quad G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}}$,

then $\quad e = r - Gd$. Then the method (40) can be written as

$$\sum_{i=0}^{k-q} \hat{\alpha}^F_{i,n} y_{n+k-i} + \sum_{i=k-q+1}^{k} \hat{\alpha}^F_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0,$$

or,

$$\sum_{i=0}^{k-q} \hat{\alpha}^F_{i,n} y_{n+k-i} + \sum_{i=k-q+1}^{k} \left(r_{i+q-k} - \sum_{j=0}^{k-q} \hat{\alpha}^F_{j,n}\, g_{i+q-k,\, j+1} \right) y_{n+k-i}$$
$$- h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0,$$

or,

$$\sum_{i=0}^{k-q} \hat{\alpha}^F_{i,n} y_{n+k-i} + \sum_{j=k-q+1}^{k} \left(r_{j+q-k} - \sum_{i=0}^{k-q} \hat{\alpha}^F_{i,n}\, g_{j+q-k,\, i+1} \right) y_{n+k-j}$$
$$- h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0;$$

or, we get

$$(46) \qquad \sum_{i=0}^{k-q} \hat{\alpha}^F_{i,n} \left(y_{n+k-i} - \sum_{j=k-q+1}^{k} g_{j+q-k,\, i+1} y_{n+k-j} \right) +$$
$$\sum_{j=k-q+1}^{k} r_{j+q-k}\, y_{n+k-j} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0$$

Hence we get the following Theorem:

Theorem 9: An optimal multistep method

$$\sum_{i=0}^{k} \hat{\alpha}^{F}_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \beta_i f_{n+k-i} = 0,$$

where β_i's are prefixed, is interpolatory for arbitrary functions $f_1, f_2, \ldots, f_q$, if and only if it is interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i : i = 0(1)k-q\},$$

where $h_i = K(x, \bar{x}_{n+k-i}) + \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1} K(x, \bar{x}_{n+k-j}),$

where r_i and g_{ij}'s are defined in (42), (44), (45).

Proof: From equation (46) we find that to determine the optimal coefficients $\hat{\alpha}^{F}_{i,n}$, $i = 0(1)k-q$, the normal equations can be obtained by minimizing the norm of the local truncation error functional $\hat{T}^{F}_{n}$ for the method (46), with respect to the coefficients $\hat{\alpha}^{F}_{i,n}$, $i = 0(1)k-q$. Thus we get the system of normal equations

$$(h_i , \hat{T}^{F}_{n}) = 0, \quad i = 0(1)k-q$$

where $h_i = K(x, \bar{x}_{n+k-i}) + \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1} K(x, \bar{x}_{n+k-j}),$

and the method (46) is also interpolatory for the functions $f_1, f_2, \ldots, f_q$. Hence the proof.

Now we shall find β-optimal multistep method interpolatory for linearly independent arbitrary functions under some restriction.

Let

(47) $$\sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n}\, f_{n+k-i} = 0$$

be the optimal multistep method interpolatory for linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$, where $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$ are the optimal coefficients to be determined subject to the condition that

(48) $$\sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n} = 1.$$

For convenience, let us write, $\hat{\beta}^F_{k,n} = 1 - \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^F_{i,n}$.

Then the method (47) becomes

(48) $$\sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^F_{i,n}\left(f_{n+k-i} - f_n\right) - h^2 f_n = 0.$$

The representer for the local truncation error functional for the method (48), in a Hilbert space possessing a reproducing kernel function is given by

$$\hat{T}^F_n = \sum_{i=0}^{k}\bar{\alpha}_i K(t,\bar{x}_{n+k-i}) - h^2\sum_{i=\delta_{t0}}^{k-1} \bar{\hat{\beta}}^F_{i,n}\left(D2(t,\bar{x}_{n+k-i}) - D2(t,\bar{x}_n)\right) - h^2 D2(t,\bar{x}_n).$$

To obtain the optimal coefficients $\hat{\beta}^F_{i,n}$, $i=\delta_{t0}(1)k-1$, we have to minimize, $\|\hat{T}^F_n\|^2$ subject to the condition $(\hat{T}^F_n, f_m) = 0$, $m = 1(1)q$. Using the methodology of Lagrange multipliers, we get the following system of equations to determine $\hat{\beta}^F_{i,n}$, $i=\delta_{t0}(1)k-1$.

(49) $$\begin{bmatrix} A & -F^* \\ F & 0 \end{bmatrix}\begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where F^* is the complex conjugate of F.

$$A = (A_{ij})_{\substack{i=\delta_{t0}(1)k-1,\\ j=\delta_{t0}(1)k-1}} \quad \text{with}$$

$$A_{ij} = D2''(x_{n+k-j},\bar{x}_{n+k-i})-D2''(x_{n+k-j},\bar{x}_n)-D2''(x_n,\bar{x}_{n+k-i})+D2''(x_n,\bar{x}_n),$$

$$F = (F_{ij})_{\substack{i=1(1)q\\ j=\delta_{t0}(1)k-1}}, \quad \text{with} \quad F_{ij}= f_i''(x_{n+k-j}) - f_i''(x_n),$$

$$b = h^2\left(\hat{\beta}^F_{\delta_{t0},n},\hat{\beta}^F_{\delta_{t0}+1,n},\ldots,\hat{\beta}^F_{k-1,n}\right)^T, \quad \lambda = (\lambda_1,\lambda_2,\ldots,\lambda_q)^T,$$

$$c = \left(c_{\delta_{t0}},c_{\delta_{t0}+1},\ldots,c_{k-1}\right)^T, \quad \text{with}$$

$$c_i = \sum_{j=0}^{k}\alpha_j\left(D2(x_{n+k-j},\bar{x}_{n+k-i})-D2(x_{n+k-j},\bar{x}_n)\right)$$

$$- h^2\left(D2''(x_n,\bar{x}_{n+k-i})-D2''(x_n,\bar{x}_n)\right), \quad \text{for} \quad i = \delta_{t0}(1)k-1,$$

and

$$f = (\tilde{f}_1,\tilde{f}_2,\ldots,\tilde{f}_q)^T, \quad \text{with } \tilde{f}_i = \sum_{j=0}^{k}\alpha_j f_i(x_{n+k-j}) - h^2 f_i(x_n).$$

If the above matrix is invertible, then the system of linear equations can be solved to have the unique solution, $\hat{\beta}^F_{i,n}$, $i=\delta_{t0}(1)k-1$.

Now we shall characterize the β-optimal multistep method interpolatory for arbitrary functions under the restriction (48). For simplicity in the form of characterization, we assume that the last p columns in the matrix (32) are linearly independent. In general, our assumption is that some p columns of the matrix (32) are linearly independent. Then in the corresponding

characterization, the indices of these columns instead of the las p columns in the simpler case would appear in the formulation.

Let the interpolatory condition appearing in (49)

$$Fb = f,$$

be rewritten as

$$[E \mid P] \begin{bmatrix} d \\ e \end{bmatrix} = f,$$

where

(50) $$E = \left(f_i''(x_{n+k-j}) - f_i''(x_n)\right)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-q-1}},$$

(51) $$P = \left(f_i''(x_{n+k-j}) - f_i''(x_n)\right)_{\substack{i=1(1)q \\ j=k-q(1)k-1}},$$

(52) $$d = \left(\hat{\beta}^F_{\delta_{t0},n}, \ldots, \hat{\beta}^F_{k-q-1,n}\right)^T, \quad e = \left(\hat{\beta}^F_{k-q,n}, \ldots, \hat{\beta}^F_{k-1,n}\right)^T,$$

(53) $f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T$, with

$$\tilde{f}_i = \frac{1}{h^2}\left(\sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j}) - h^2 f_i(x_n)\right).$$

Then $e = P^{-1}(f - Ed)$. Let

(54) $$r = P^{-1}f = (r_0, r_1, \ldots, r_{q-1})^T,$$

(55) $$G = P^{-1}E = (g_{ij})_{\substack{i=0(1)q-1 \\ j=1(1)k-q-\delta_{t0}}};$$

then $e = r - Gd$. Then the method (48) can be written as

$$\sum_{i=0}^{k} \alpha_i y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-q-1} \hat{\beta}^F_{i,n}\left(f_{n+k-i} - f_n\right) - h^2 \sum_{i=k-q}^{k-1} \hat{\beta}^F_{i,n}\left(f_{n+k-i} - f_n\right) - h^2 f_n = 0,$$

$$\text{or,}\quad \sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k-q-1}\hat{\beta}^F_{i,n}\left(f_{n+k-i}-f_n\right) - h^2 f_n$$

$$- h^2\sum_{i=k-q}^{k-1}\left(r_{i+q-k} - \sum_{j=\delta_{t0}}^{k-q-1}\hat{\beta}^F_{j,n}\, g_{i+q-k,\, j+1-\delta_{t0}}\right)\left(f_{n+k-i}-f_n\right) = 0,$$

or,

$$(56)\qquad \sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=k-q}^{k-1} r_{i+q-k} f_{n+k-i} - h^2 f_n$$

$$- h^2\sum_{i=\delta_{t0}}^{k-q-1}\hat{\beta}^F_{i,n}\left(\{f_{n+k-i} - f_n\} - \sum_{j=k-q}^{k-1} g_{j+q-k,\, i+1-\delta_{t0}} f_{n+k-j}\right) = 0.$$

Hence we get the following Theorem:

Theorem 10: The optimal multistep method,

$$\sum_{i=0}^{k}\alpha_i y_{n+k-i} - h^2\sum_{i=\delta_{t0}}^{k}\hat{\beta}^F_{i,n}\, f_{n+k-i} = 0,$$

where α_i's are prefixed and $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$ are the optim coefficients to be determined subject to the condition

$$\sum_{i=\delta_{t0}}^{k}\hat{\beta}^F_{i,n} = 1,$$

is interpolatory for arbitrary functions $f_1, f_2, \ldots, f_q$; if and only if it is interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i : i = \delta_{t0}(1)k-q-1\},$$

where $h_i = D2(x, \bar{x}_{n+k-i}) - D2(x, \bar{x}_n)$

$$- \sum_{j=k-q}^{k-1} \bar{g}_{j+q-k,\, i+1-\delta_{t0}} \left(D2(x, \bar{x}_{n+k-j}) - D2(x, \bar{x}_n) \right),$$

with g_{ij}'s defined by (55), (50), (51).

Proof: From equation (56), we see that to determine the optim coefficients $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k-q-1$ the normal equations can obtained by minimizing the norm of the local truncation err functional $\hat{T}^F_n$ for the method (56), with respect to the coefficien $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k-q-1$. Thus we get the system of normal equations

$$(h_i \; , \; \hat{T}^F_n) = 0, \quad i = \delta_{t0}(1)k-q-1,$$

where $h_i(x) = D2(x, \bar{x}_{n+k-i}) - D2(x, \bar{x}_n)$

$$- \sum_{j=k-q}^{k-1} \left(\bar{g}_{j+q-k,\, i+1-\delta_{t0}} D2(x, \bar{x}_{n+k-j}) - D2(x, \bar{x}_n) \right),$$

and the method (56) is also interpolatory for the functio $f_1, f_2, \ldots, f_q$. Hence the proof.

Now we shall find α as well as β-optimal multistep meth interpolatory for linearly independent arbitrary functions und some restriction.

Let

(57) $$\sum_{i=0}^{k} \hat{\alpha}^F_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n} \; f_{n+k-i} = 0$$

be the optimal method interpolatory for arbitrary functions f $f_2, \ldots, f_q$, where $\hat{\alpha}^F_{i,n}$, $i = 0(1)k$ and $\hat{\beta}^F_{i,n}$, $i = \delta_{t0}(1)k$ are t optimal coefficients to be determined subject to the condition

$$(58)\qquad \sum_{i=\delta_{t0}}^{k} \hat{\beta}^F_{i,n} = 1.$$

For convenience, let us write

$$\hat{\beta}^F_{k,n} = 1 - \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^F_{i,n}.$$

Then the method (57) becomes

$$(59)\qquad \sum_{i=0}^{k} \hat{\alpha}^F_{i,n} y_{n+k-i} - h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^F_{i,n}\left(f_{n+k-i} - f_n\right) - h^2 f_n = 0.$$

The representer for the local truncation error functional for th method (59) in a Hilbert space possessing a reproducing kerne function is given by

$$\hat{T}^F_n = \sum_{i=0}^{k} \bar{\hat{\alpha}}^F_{i,n} K(t,\bar{x}_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k-1} \bar{\hat{\beta}}^F_{i,n}\left(D2(t,\bar{x}_{n+k-i}) - D2(t,\bar{x}_n)\right) - h^2 D2(t,\bar{x}_n).$$

To obtain the optimal coefficients $\hat{\alpha}^F_{i,n}$, $i=0(1)k$ and $\hat{\beta}^F_{i,n}$ $i=\delta_{t0}(1)k-1$, at a point x_n, we have to minimize, $\|\hat{T}^F_n\|^2$ subject t the condition $(\hat{T}^F_n\ ,\ f_m) = 0$, $m = 1(1)q$. Thus we get the followin system of linear equations

$$(60)\qquad \sum_{i=0}^{k} \hat{\alpha}^F_{i,n} K(x_{n+k-l},\bar{x}_{n+k-i})$$

$$- h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^F_{i,n}\left(\overline{D2(x_{n+k-l},\bar{x}_{n+k-i})} - \overline{D2(x_{n+k-l},\bar{x}_n)}\right) + \sum_{m=1}^{q} \lambda_m \overline{f_m(x_{n+k-l})}$$

$$= h^2\overline{D2(x_{n+k-l},\bar{x}_n)}, \qquad l = 0(1)k$$

$$(61) \qquad \sum_{i=0}^{k} \hat{\alpha}^{F}_{i,n} \left(D2(x_{n+k-i}, \bar{x}_{n+k-1}) - D2(x_{n+k-i}, \bar{x}_{n}) \right)$$

$$- h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^{F}_{i,n} \Big(D2''(x_{n+k-i}, \bar{x}_{n+k-1}) - D2''(x_{n+k-i}, \bar{x}_{n})$$

$$- D2''(x_{n}, \bar{x}_{n+k-1}) + D2''(x_{n}, \bar{x}_{n}) \Big) + \sum_{m=1}^{q} \lambda_m \left(\overline{f''_m(x_{n+k-1})} - \overline{f''_m(x_n)} \right)$$

$$= h^2 \left(D2''(x_{n}, \bar{x}_{n+k-1}) - D2''(x_{n}, \bar{x}_{n}) \right), \qquad l = \delta_{t0}(1)k-1.$$

Since method (59) is interpolatory for the functions f_m; $m = 1(1)q$

$$(62) \quad \sum_{i=0}^{k} \hat{\alpha}^{F}_{i,n} f_m(x_{n+k-i}) - h^2 \sum_{i=\delta_{t0}}^{k-1} \hat{\beta}^{F}_{i,n} \left(f''_m(x_{n+k-i}) - f''_m(x_n) \right) = h^2 f''_m(x_n),$$

$$m = 1(1)q.$$

Solving the system of equations (60), (61) and (62) we ca find the optimal coefficients $\hat{\alpha}^{F}_{i,n}$, $i = 0(1)k$ and $\hat{\beta}^{F}_{i,n}$, i $\delta_{t0}(1)k-1$.

CHAPTER 2

ERROR ANALYSIS OF THE OPTIMAL LINEAR MULTISTEP METHODS FOR INITIAL VALUE PROBLEM FOR SECOND ORDER DIFFERENTIAL EQUATION

2.1 Introduction

This chapter is a study of certain theoretical aspects of the β-optimal linear multistep methods where optimization is done with respect to β coefficients with prefixed α's and a linear multistep method with mildly varying coefficients, implemented for an initial value problem. These aspects concern convergence analysis, magnitude of discretization error, propagation of round off error and stability analysis. The study also includes the β - optimal multistep methods which are interpolatory for polynomials of certain degree and other functions.

The results for the β-optimal methods, obtained in this chapter establish the applicability of the β-optimal methods to a general situation in which the solution does not necessarily belong to the underlying Hilbert space.

The space of optimization for the β-optimal multistep methods is H, say. The interval [a,b] of integration is a subset of the open interval (-r,r), for the Hilbert spaces $H^2(C_r)$ or $L^2(\hat{C}_r)$. The nodal points x_i's satisfy the relation $a = x_0 < x_1 < x_2 < \dots < x_N = b$ and they are equispaced with spacing h, with $Nh = b-a$. For the β-optimal multistep methods the optimal coefficients β_j's will depend on the current variable x_n in the integration scheme. The

dependence of β_j's on the point x_n is indicated by writing them as $\beta_{j,n}$'s.

In section 2.2, we state some results from Henrici [96], which we shall use in the subsequent sections. In section 2.3, we have given an estimate of local truncation error for the β-optimal multistep methods. In section 2.4, we state the relation between the optimal β-coefficients and the usual β-coefficients as $h \to 0$. In section 2.5, convergence of the β-optimal multistep method has been established. In sections 2.6 and 2.7, a bound of discretization error and a bound of propagation of round off error have been derived.

In the following sections we have also discussed about a linear multistep method with mildly varying coefficients. Using a linear multistep method with mildly varying coefficients, instead of using a linear multistep method with constant coefficients, we might not necessarily complicate the situation; rather we may gain something more. For example, for a weakly stable linear multistep method with constant coefficients, the numerical solution of the method might have uncontrolled growth. However, the growth of the numerical solution of the corresponding linear multistep method with mildly varying coefficients, could be controlled.

In section 2.8, we have established the convergence of a linear multistep method with mildly varying coefficients. In section 2.9, we have given an estimate of local truncation error for this method. In sections 2.10 and 2.11, a bound for discretization error and a bound for propagation of round off error of this method have been derived. In section 2.12, solution of

error equation of this method is derived and some criteria of stability of this method have been discussed.

We consider the following class of initial value problem for a special second order differential equation

(1) $$y'' = f(x,y); \quad y(a) = \eta,\ y'(a) = \eta',$$

on an interval $a \le x \le b$, where the function $f(x,y)$ satisfies the conditions (i) and (ii) stated in section 1.1.

A general linear k-step method for the numerical solution of the initial value problem (1) is given by

(2) $$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f_{n+j}$$

where $y_j = y(x_j)$, $f_j = f(x_j, y_j)$, $x_j = a+jh$, $j = 0(1)N$, α_j, β_j, $j = 0(1)k$, are real constants with $\alpha_k \neq 0$, and $|\alpha_j| + |\beta_j| \neq 0$. If $\beta_k = 0$, the method (2) is an explicit method, and if $\beta_k \neq 0$, the method is an implicit one.

2.2 Some Well Known Results for the Usual Method

In this section, we shall state some well known results for the usual linear multistep methods for an initial value problem of the form (1), which are used in the analysis in the following sections. Let

(3) $$L\,[y(x);h] = \sum_{i=0}^{k} \alpha_i y(x+ih) - h^2 \sum_{i=0}^{k} \beta_i y''(x+ih)$$

be the difference operator associated with the difference eqn. (2). Let $L\,[y(x);h]$ be applied to functions which have continuous derivatives of sufficiently high order. Then expanding in powers of

h, we obtain

$$L\,[y(x);h] = C_0 y(x) + C_1 y'(x)h + \dots\dots\dots + C_q y^{(q)}(x)h^q + \dots\dots,$$

where the coefficients C_q $(q = 1,2,\dots.)$ are independent of $y(x)$ and are given by the following expressions.

$$C_0 = \sum_{i=0}^{k} \alpha_i, \quad C_1 = \sum_{i=1}^{k} i\alpha_i \;,$$

and $$C_q = \frac{1}{q!}\sum_{i=1}^{k} i^q\alpha_i - \frac{1}{(q-2)!}\sum_{i=0}^{k} i^{q-2}\beta_i, \quad q=2,3,\dots\dots .$$

<u>Definition 1:</u> The order p of the difference operator (3) is defined as the unique integer such that $C_q = 0$, $q = 0,1,\dots.p+1$; $C_{p+2} \neq 0$.

<u>Lemma 1:</u> (Henrici [96]) Let $L\,[y(x);h]$ be a difference operator of order $p > 0$. There exists a constant $G > 0$, depending only on L, such that

$$|L[y(x);h]| \le h^{p+2}GY, \quad a \le x, \quad x+kh \le b,$$

for all functions $y(x)$ having a continuous derivatives of order $p+2$ in $[a,b]$, where $Y = \max_{a\le x\le b} |\, y^{(p+2)}(x) \,|$.

<u>Definition 2:</u> (Henrici [96]) The linear multistep method defined by (2) is called convergent if the following statement is true for all functions $f(x,y)$ satisfying the conditions (i) and (ii) stated in section 1.1 and all constants η and η':

If $y(x)$ denotes the solution of the initial value problem

$$y'' = f(x,y) \;; \quad y(a) = \eta, \; y'(a) = \eta'$$

then

$$\lim_{\substack{h \to 0 \\ x_n = x}} y_n = y(x)$$

holds for all $x \in [a,b]$, and for all sequences $\{y_n\}$ defined by (2) with starting values

$$y_\mu = \eta_\mu(h), \; \mu = 0,1,2,\ldots.k-1,$$

satisfying the following two conditions

$$\lim_{h \to 0} \eta_\mu(h) = \eta, \qquad \mu = 0,1,2,\ldots.k-1,$$

$$\lim_{h \to 0} \frac{\eta_\mu(h)-\eta_0(h)}{\mu h} = \eta', \qquad \mu = 0,1,2,\ldots.k-1.$$

With the difference equation (2) or with the difference operator (3) we can associate the polynomials

$$\rho(\zeta) = \sum_{i=0}^{k} \alpha_i \zeta^i, \quad \text{and} \quad \sigma(\zeta) = \sum_{i=0}^{k} \beta_i \zeta^i.$$

<u>Theorem 1:</u> (Theorem 6.1, Henrici [96]) A necessary condition for the convergence of the linear multistep method (2) is that the modulus of no root of the polynomial $\rho(\zeta)$ exceeds 1, and that the multiplicity of the roots of modulus 1 be atmost 2.

The condition thus imposed on the roots of $\rho(\zeta)$ is called the condition of stability.

<u>Theorem 2:</u> (Theorem 6.2, Henrici [96]) The order of a convergent linear multistep method (2) is at least 1.

This condition is called the condition of consistency.

The condition of consistency demands that the constants C_i's

defined earlier should satisfy $C_0 = C_1 = C_2 = 0$, or in other words

$$\rho(1) = 0, \quad \rho'(1) = 0, \quad \rho''(1) = 2\sigma(1).$$

Lemma 2: (Lemma 6.2, Henrici [96]) Let the polynomial $\rho(\zeta) = \alpha_k\zeta^k + \ldots\ldots + \alpha_0$ satisfy the condition of stability for the integration of second order differential equation, and let the coefficients γ_l ($l = 0,1,2,\ldots.$) be defined by

$$(4) \qquad \frac{1}{\alpha_k + \alpha_{k-1}\zeta + \ldots + \alpha_0\zeta^k} = \gamma_0 + \gamma_1\zeta + \gamma_2\zeta^2 + \ldots\ldots .$$

Then there exist two constants Γ and γ such that

$$(5) \qquad |\gamma_l| \le l\Gamma + \gamma, \qquad l = 0,1,2,\ldots. .$$

The following lemma is for the growth of the solution of the difference equation of the form

$$(6) \qquad \alpha_k z_{m+k} + \alpha_{k-1} z_{m+k-1} + \ldots + \alpha_0 z_m$$

$$= h^2(\beta_{k,m} z_{m+k} + \beta_{k-1,m} z_{m+k-1} + \ldots + \beta_{0,m} z_m) + \lambda_m.$$

Lemma 3: (Lemma 6.3, Henrici [96]) Let the polynomial $\rho(\zeta) = \alpha_k\zeta^k + \ldots\ldots + \alpha_0$ satisfy the condition of stability for the integration of second order differential equation, and let B^*, β and Λ be constants such that

$$(7) \qquad |\beta_{k,m}| + |\beta_{k-1,m}| + \ldots + |\beta_{0,m}| \le B^*, \qquad |\beta_{k,m}| \le \beta, \qquad |\lambda_m| \le \Lambda;$$

for $0 \le m \le N$,

and let $0 \le h^2 < |\alpha_k|\beta^{-1}$. Then every solution of the difference equation (6) for which

$$(8) \qquad |z_\mu| \le Z, \qquad \mu = 0,1,2,\ldots\ldots,k-1$$

satisfies

(9) $$|z_n| \le K^* \exp\{nh^2 L^*\}, \qquad 0 \le n \le N.$$

Here

(10) $$L^* = \frac{(N\Gamma + \gamma)B^*}{1 - h^2|\alpha_k^{-1}|\beta}, \quad \text{and} \quad K^* = \frac{(\frac{1}{2} N^2\Gamma + N\gamma)A + (N\Gamma + \gamma)kAZ}{1 - h^2|\alpha_k^{-1}|\beta},$$

where $A = |\alpha_k| + |\alpha_{k-1}| + \ldots\ldots + |\alpha_0|$, and Γ and γ are defined by (5).

<u>Theorem 3:</u> (Theorem 6.6, Henrici [96]) The linear multistep method defined by (2) is convergent if and only if it satisfies the conditions of stability and consistency.

2.3 <u>Optimal Multistep Methods for Initial Value Problems</u>

In the following sections we shall obtain an error analysis of the optimal multistep methods when the α-coefficients are kept fixed and the β-coefficients are optimized in a Hilbert space H, say.

<u>Lemma 4:</u> Let

$$L[y(x);h] = \sum_{j=0}^{k} \alpha_{k-j} y(x+(k-j)h) - h^2 \sum_{j=\delta_{t0}}^{k} \beta_{k-j} y''(x+(k-j)h)$$

be the difference operator of a k-step usual multistep method of order $p > 0$, and let

$$\hat{L}[y(x);h] = \sum_{j=0}^{k} \alpha_{k-j} y(x+(k-j)h) - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,x} y''(x+(k-j)h)$$

be the difference operator of the corresponding optimal method, where $\hat{\beta}_{k-j,x}$; $0 \le j \le k$, are the optimal coefficients depending on x, corresponding to the usual coefficients β_{k-j}, $0 \le j \le k$. Let the

exact solution $y(x)$ of the differential equation have a continuous derivatives of order p+2 for $x \in [a,b]$ and let

$$Y = \max_{\substack{a \le x \le b \\ 0 \le i \le p+2}} |y^{(i)}(x)|.$$

Then in a Hilbert space, H, in which D_x^{p+2}, the representer of p+2-th derivative evaluation functional at x exists and is uniformly bounded in [a,b],

$$|\hat{L}[y(x);h]| \le h^{p+2} G^* Y, \quad a \le x, \quad x+kh \le b.$$

where G^* is a positive constant.

<u>Proof:</u> If $y(x)$ has a continuous derivative of order p+2 in [a,b] and if x and $\bar{x}$ are in [a,b] then by Taylor's theorem with the integral form of the remainder, $y(x) = P(x) + Q(x)$, say, where

$$P(x) = y(\bar{x}) + (x-\bar{x})y'(\bar{x}) + \dots \quad \dots + \frac{(x-\bar{x})^{p+1}}{(p+1)!} y^{(p+1)}(\bar{x}),$$

and

$$Q(x) = \frac{1}{(p+1)!} \int_{\bar{x}}^{x} (x-t)^{p+1} \, y^{(p+2)}(t)\,dt.$$

Let $\| L \|$ and $\| \hat{L} \|$ denote the norms of the difference operators L and $\hat{L}$, respectively. Then since in the space of optimization, $\| \hat{L} \| \le \| L \|$, we get

$$(11) \qquad | \hat{L}[P(x);h] | \le \| \hat{L} \| \, \| P \|$$

$$\le \| L \| \, \| P \|$$

$$\le (C_1 M_{p+2} h^{p+2}) \; (C_2 Y),$$

using Lemma 1, where

$$M_{p+2} = \max_{a \le x \le b} \| D_x^{p+2} \|,$$

D_x^{p+2} being the linear operator for the (p+2)-th derivative, C_1 and C_2 are positive constants independent of x. Again

$$(12) \qquad \begin{aligned} | \hat{L}[Q(x);h] | &\le \| \hat{L} \| \, \| Q \| \\ &\le \| L \| \, \| Q \| \\ &\le (C_1 M_{p+2} h^{p+2}) \; (C_3 Y), \end{aligned}$$

using Lemma 1, where C_3 is a positive constant. Then since, $\hat{L}$ is a linear operator, using (11), and (12), we get

$$\begin{aligned} | \hat{L}[y(x);h] | = | \hat{L}[P(x)+Q(x);h] | &= | \hat{L}[P(x);h] + \hat{L}[Q(x);h] | \\ &\le | \hat{L}[P(x);h] | + | \hat{L}[Q(x);h] | \\ &\le C_1(C_2+C_3)M_{p+2}h^{p+2}Y. \end{aligned}$$

So, $| \hat{L}[y(x);h] | \le G^* h^{p+2} Y$, where $G^* = C_1(C_2+C_3)M_{p+2}$ is a positive constant. Hence the proof.

2.4 Relation Between Optimal and Usual β-Coefficients.

The following lemma relates the coefficients of the β-optimal multistep method to those of the corresponding usual multistep method.

Lemma 5 : Let

$$(13) \qquad \sum_{j=0}^{k} \alpha_{k-j} y_{n+k-j} = h^2 \sum_{j=\delta_{t0}}^{k} \beta_{k-j} f(x_{n+k-j}, y_{n+k-j}), \qquad 0 \le n \le N-k,$$

be a usual method of order p with constant coefficients α_{k-j}'s and

β_{k-j}'s. Let

$$(14) \qquad \sum_{j=0}^{k} \alpha_{k-j} y_{n+k-j} = h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,n} f(x_{n+k-j}, y_{n+k-j}), \qquad 0 \le n \le N-k$$

be the corresponding β-optimal method. Then in a Hilbert space, H, in which D_x^{p+2}, the representer of (p+2)-th derivative evaluation functional at $x \in [a,b]$ exists and is uniformly bounded in [a,b],

$$|\hat{\beta}_{j,n} - \beta_j| = O(h^{p-k+\delta_{t0}}), \quad h \to 0, \quad j = \delta_{t0}(1)k,$$

uniformly for every n, $0 \le n \le N-k$.

<u>Proof</u>: Let us consider the polynomials

$$l_{i,n}(x) = \prod_{\substack{j=\delta_{t0} \\ j \ne i}}^{k} \frac{(x - x_{n+k-j})}{(x_{n+k-i} - x_{n+k-j})}, \quad i = \delta_{t0}(1)k, \quad 0 \le n \le N-k,$$

of degree $k - \delta_{t0}$. As x_{n+k-j}'s are in [a,b] and are equispaced,

$$\| l_{i,n} \| = O\,(h^{-(k-\delta_{t0})}), \qquad \text{uniformly in } i \text{ and } n.$$

Let $M_{i,n}(x)$ be a function which satisfies the differential equation

$$M''_{i,n}(x) = l_{i,n}(x), \qquad i = \delta_{t0}(1)k; \quad 0 \le n \le N-k,$$

and the initial conditions $M_{i,n}(a) = M'_{i,n}(a) = 0$. Then

$$M'_{i,n}(x) = \int_a^x l_{i,n}(u)\, du = F_{i,n}(x), \text{ say,}$$

and $$M_{i,n}(x) = \int_a^x F_{i,n}(u)\, du, \qquad i = \delta_{t0}(1)k; \quad 0 \le n \le N-k.$$

and $M_{i,n}(x)$ is a polynomial of degree $k+2-\delta_{t0}$ and

$$(15) \qquad \| M_{i,n} \| = O\,(h^{-(k-\delta_{t0})}), \qquad \text{uniformly in } i \text{ and } n.$$

Since the usual method (13) is exact for polynomials of degree

p+1, it will be exact for $M_{i,n}(x)$, $i = \delta_{t0}(1)k$, if $p+1 \geq k+2-\delta_{t0}$. Hence

$$\sum_{j=0}^{k} \alpha_{k-j}\, M_{i,n}(x_{n+k-j}) = h^2 \sum_{j=\delta_{t0}}^{k} \beta_{k-j}\, l_{i,n}(x_{n+k-j}).$$

Since $l_{i,n}(x_{n+k-j}) = \delta_{ij}$, $0 \leq n \leq N-k$, we get

$$\sum_{j=0}^{k} \alpha_{k-j}\, M_{i,n}(x_{n+k-j}) = h^2\beta_{k-i}, \quad i = \delta_{t0}(1)k. \tag{16}$$

Let $L[y(x);h]$ and $\hat{L}[y(x);h]$ be the difference operators associated with the usual method (13) and the optimal method (14) respectively which represent for the local truncation error functionals of these methods. Now by applying the optimal method (14) on $M_{i,n}(x)$, and using (16) and the fact that $\|\hat{L}\| \leq \|L\|$, in H, we get

$$\left| \sum_{j=0}^{k} \alpha_{k-j}\, M_{i,n}(x_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,n} l_{i,n}(x_{n+k-j}) \right| = |\hat{L}[M_{i,n};h]|,$$

or,
$$\left| \sum_{j=0}^{k} \alpha_{k-j}\, M_{i,n}(x_{n+k-j}) - h^2\hat{\beta}_{k-i,n} \right| \leq \|\hat{L}\|\ \|M_{i,n}\|,$$

or,
$$|h^2\beta_{k-i} - h^2\hat{\beta}_{k-i,n}| \leq \|L\|\ \|M_{i,n}\|$$

$$h^2|\beta_{k-i} - \hat{\beta}_{k-i,n}| \leq Ch^{p+2}M_{p+2}\|M_{i,n}\|,$$

where $M_{p+2} = \max \|D_x^{p+2}\|$, D_x^{p+2} being the representer of (p+2)-th derivative evaluation functional. Using (15) we get

$$|\hat{\beta}_{i,n} - \beta_i| = O(h^{p-k+\delta_{t0}}), \quad h \to 0,\ i = \delta_{t0}(1)k,$$

uniformly for every n, $0 \leq n \leq N-k$. Hence the proof.

Remark: It is easily seen that if only q of the β_i's are nonzero and are being optimized, we have instead the estimate

$$|\hat{\beta}_{i,n} - \beta_i| = O(h^{p-q+1}), \quad h \to 0, \ i = \delta_{t0}(1)k,$$

uniformly for every n, $0 \le n \le N-k$.

Some examples are given below:

(i) For Cowell's method with function evaluation at three points:

$$y_{n+1} - 2y_n + y_{n-1} = h^2\{1/12\ f_{n+1} + 10/12 f_n + 1/12 f_{n-1}\},$$

we have p = 4, q = 3, so, $|\hat{\beta}_{i,n} - \beta_i| = O(h^2)$, $h \to 0$, $i = 0(1)2$.

(ii) For Stormer's method with function evaluation at one point:

$$y_{n+1} - 2y_n + y_{n-1} = h^2 f_n,$$

we have p = 2, q = 1, so, $|\hat{\beta}_{1,n} - \beta_1| = O(h^2)$, $h \to 0$.

(iii) For Stormer's method with function evaluation at five points:

$$y_{n+1} - 2y_n + y_{n-1} = h^2[\frac{299}{240}f_n - \frac{11}{15}f_{n-1} + \frac{97}{120}f_{n-2} - \frac{2}{5}f_{n-3} + \frac{19}{240}f_{n-4}],$$

we have p = 5, q = 5, so, $|\hat{\beta}_{i,n} - \beta_i| = O(h)$, $h \to 0$, $i = 0(1)4$.

(iv) For a difference method of the form:

$$- y_{n-1} + y_n + y_{n+1} - y_{n+2} + 2h^2 f_{n-1} = 0,$$

we have p = 1, q = 1, so, $|\hat{\beta}_{0,n} - \beta_0| = O(h)$, $h \to 0$.

Assuming that $p-k+\delta_{t0} \ge 1$, in the following section, we are establishing the convergence theorem using $|\hat{\beta}_{i,n} - \beta_i| = O(h)$.

2.5 Convergence of β-Optimal Methods

Theorem 4 : In a Hilbert space H, in which D_x^{p+2}, the representer of (p+2)-th derivative evaluation functional at x exists and is

niformly bounded in [a,b], the k-step β-optimal multistep method 14), corresponding to a stable and consistent usual multistep ethod (13), is convergent.

roof: Let the function $f(x,y)$ satisfy the conditions (i) and ii) given in section 1.1 and let η be an arbitrary constant. Let (x) be the solution of the initial value problem (1). Let y_n, $0 \le n$ N-k be the solution of the difference equation (14) defined by the starting values $y_\mu = \eta_\mu(h)$, $0 \le \mu \le k-1$. We set the initial error

$$h\delta(h) = \max_{0 \le \mu \le k-1} | \eta_\mu(h) - y(a+\mu h) |,$$

here $\delta(h) \to 0$ as $h \to 0$.

Let $L[y(x);h]$ and $\hat{L}[y(x);h]$ be the difference operators ssociated with the usual method (13) and the optimal method (14) respectively, for the point $x = x_m$, $0 \le m \le N-k$. Let

$$\| y'' \| = \max_{x \in [a,b]} | y''(x) |.$$

Jsing Lemma 5, we get for the point $x = x_m$,

$$|\hat{L}[y(x_m);h] - L[y(x_m);h]| = \left| h^2 \sum_{j=\delta_{t0}}^{k} (\hat{\beta}_{k-j,m} - \beta_{k-j}) y''(x_{m+k-j}) \right|$$

$$\le h^2 \| y'' \| \sum_{j=\delta_{t0}}^{k} |\hat{\beta}_{k-j,m} - \beta_{k-j}| = O(h^3).$$

Since L is consistent,

$$| L[y(x_m);h] | = o(h^2).$$

So, $\quad | \hat{L}[y(x_m);h] | \le | L[y(x_m);h] | + O(h^3) = o(h^2),$

or, $\quad | \hat{L}[y(x_m);h] | = \theta_m h^2 \theta(h),$

ıere $|\theta_m| \le 1$, and $\theta(h) \to 0$ as $h \to 0$. Thus we get for $0 \le m \le N-k$,

$$\text{L7)}\quad \sum_{j=0}^{k} \alpha_{k-j} y(x_{m+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} f(x_{m+k-j}, y(x_{m+k-j})) = \theta_m h^2 \theta(h).$$

ıe numerical solution satisfies the following relation at x_m

$$18)\quad \sum_{j=0}^{k} \alpha_{k-j} y_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} f(x_{m+k-j}, y_{m+k-j}) = 0.$$

Let

$$19)\quad e_m = y_m - y(x_m), \quad 0 \le m \le N-k, \quad \text{and}$$

$$20)\quad g_m = \begin{cases} [f(x_m,y_m) - f(x_m,y(x_m))]e_m^{-1}, & \text{if } e_m \ne 0, \\ 0, & \text{if } e_m = 0. \end{cases}$$

ubtracting (18) from (17), we get the error equation

$$21)\quad \sum_{j=0}^{k} \alpha_{k-j} e_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} g_{m+k-j} e_{m+k-j} = \theta_m h^2 \theta(h).$$

ıy Lipchitz condition (ii) of f, given in section 1.1,

$g_m| \le L$, $0 \le m \le N-k$. Now we can apply Lemma 3, with

$$;_m = e_m, \quad Z = h\,\delta(h), \quad \Lambda = h^2\theta(h), \quad N = (x_m - a)h^{-1}, \quad A = \sum_{j=0}^{k} |\alpha_{k-j}|,$$

$$\beta_{k-j,m} = \hat{\beta}_{k-j,m} g_{m+k-j}, \quad j=\delta_{t0}(1)K, \quad \beta = \sup_{m,h} |\hat{\beta}_{k,m}|,$$

$$B = \sup_{m,h} \sum_{j=\delta_{t0}}^{k} |\hat{\beta}_{k-j,m}| < \infty, \quad \sum_{j=\delta_{t0}}^{k} |\beta_{k-j,m}| = \sum_{j=\delta_{t0}}^{k} |\hat{\beta}_{k-j,m}|\,|g_{m+k-j}| \le BL.$$

For a later use, let us also put

$$22)\quad B^* = BL.$$

Then $|\beta_{k,m}| = |\hat{\beta}_{k,m} g_{m+k}| \le L|\hat{\beta}_{k,m}| \le \beta L$. Let

(23) $$\Gamma^* = \Gamma\, [1 - h^2 L|\alpha_k^{-1}|\beta]^{-1}, \quad a^* = a - h\gamma\Gamma^{-1},$$

then $\frac{1}{2} N^2\Gamma + N\gamma \le \frac{1}{2} (x_n - a^*)^2\Gamma h^{-2}$, and $N\Gamma + \gamma = (x_n - a^*)\Gamma h^{-1}$.

Thus for $h^2 < |\alpha_k| L^{-1}\beta^{-1}$, we get

$$|e_n| \le \Gamma^* \Big((x_n - a^*)kA\ \delta(h) + \frac{1}{2} (x_n - a^*)^2\theta(h)\Big)\exp\Big\{(x_n - a^*)^2\Gamma^* B^*\Big\}.$$

Since $\delta(h) \to 0$ and $\theta(h) \to 0$ as $h \to 0$, $e_n \to 0$ as $h \to 0$. This completes the proof.

2.6 A Bound for the Discretization Error

Let us assume that the exact solution $y(x)$ has a continuous derivative of order $p+2$ for $x \in [a,b]$. Set

(24) $$Y = \max_{a \le x \le b} |\, y^{(p+2)}(x)\, |.$$

Instead of the difference equation (14), let the numerical solution y_n satisfy the following equation, incorporating round offs:

(25) $$\sum_{j=0}^{k} \alpha_{k-j} y_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} f(x_{m+k-j}, y_{m+k-j}) = \theta_m K h^{q+2}, \quad 0 \le m \le N-k,$$

where $|\theta_m| \le 1$, and K, q are constants with $q > 0$. The term involving K stands for small error in the implementation of the difference scheme. Let us set the initial errors

(26) $$|y_\mu - y(x_\mu)| \le h\delta(h), \quad \mu = 0(1)k-1.$$

Theorem 5 : Under the conditions (24), (25) and (26), if $h^2 < |\alpha_k|\ L^{-1}\beta^{-1}$, the discretization error, $e_n = y_n - y(x_n)$, satisfies

$$|e_n| \le \Gamma^*\left[(x_n-a^*)kA\delta(h)+\frac{1}{2}(x_n-a^*)^2\{Kh^q+G^*Yh^p\}\right]\exp\left\{(x_n-a^*)^2\Gamma^*B^*\right\},$$

for $a \le x_n \le b$, where Γ^*, a^* are defined in (23), B^* is defined in (22), p is the order of the difference operator $L[y(x);h]$ associated with the usual method (13), G^* is a constant depending only on $\hat{L}[y(x);h]$, the difference operator associated with the optimal method (14).

Proof: The exact solution $y(x)$ satisfies the following relation at the point x_m

$$\text{(27)}\quad \sum_{j=0}^{k}\alpha_{k-j}y(x_{m+k-j})-h^2\sum_{j=\delta_{t0}}^{k}\hat{\beta}_{k-j,m}f(x_{m+k-j},y(x_{m+k-j}))=\hat{T}_m,\quad 0\le m\le N-k,$$

where $\hat{T}_m$ is the local truncation error at the point x_m for the optimal method (14). By Lemma 4,

$$|\ \hat{T}_m\ | \le G^*Yh^{p+2}.$$

Hence, $\hat{T}_m = \theta_{m1}G^*Yh^{p+2}$, where $|\ \theta_{m1}\ | \le 1$. Let e_m and g_m be defined by (19) and (20). Subtracting (27) from (25), we get the error equation

$$\text{(28)}\quad \sum_{j=0}^{k}\alpha_{k-j}e_{m+k-j} - h^2\sum_{j=\delta_{t0}}^{k}\hat{\beta}_{k-j,m}g_{m+k-j}e_{m+k-j} = \theta'_m(Kh^{q+2}+G^*Yh^{p+2}),$$

where $|\ \theta'_m\ | \le 1$. Now applying Lemma 3 to the difference equation (28), proceed as in the proof of Theorem 4, with the only exception that $\Lambda = Kh^{q+2}+G^*Yh^{p+2}$. Then for $h^2<|\alpha_k|L^{-1}\beta^{-1}$, we get the following relation:

$$|e_n| \le \Gamma^* \Big[(x_n - a^*) kA\delta(h) + \tfrac{1}{2}(x_n - a^*)^2 \{Kh^q + G^* Yh^p\}\Big] \exp\Big\{(x_n - a^*)^2 \Gamma^* B^*\Big\}.$$

Remark: If $\delta(h) = O(h^p)$ and $q \ge p$, then $e_n = O(h^p)$.

2.7 An A-Priori Bound for Round-Off Error

Let $\tilde{y}_n$ denote the numerical solution in the presence of round-offs corresponding to the exact numerical solution y_n. Let ε_n denote the round-off in the difference equation related with $\tilde{y}_n$.

Theorem 6: If $h^2 < |\alpha_k| L^{-1} \beta^{-1}$, the round-off error $r_n = \tilde{y}_n - y_n$ satisfies for $a \le x_n \le b$,

$$|r_n| \le \varepsilon h^{-2} \Gamma^* \, \tfrac{1}{2}(x_n - a^*)^2 \exp\Big((x_n - a^*)^2 \Gamma^* B^*\Big), \qquad 0 \le n \le N-k,$$

where Γ^* and a^* are defined in (23), B^* is defined in (22), L is Lipchitz constant for the function f(x,y) and ε is a bound for local round-off errors.

Proof: The numerical approximation $\tilde{y}_m$ to y_m, the exact solution of the difference equation (14), satisfies the following equation

$$(29) \quad \sum_{j=0}^{k} \alpha_{k-j} \tilde{y}_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} f(x_{m+k-j}, \tilde{y}_{m+k-j}) = \varepsilon_{m+k}, \qquad 0 \le m \le N-k,$$

where ε_{m+k} is the local round-off, which depends on the computational procedure and on the organization of the arithmetic unit of the computing equipment. Let $|\varepsilon_m| \le \varepsilon$, where ε is independent of m.

Let $r_m = \tilde{y}_m - y_m$ be the accumulated round-off error at the point x_m, and let

$$g_m = \begin{cases} r_m^{-1}\,[f(x_m,\tilde{y}_m) - f(x_m,y_m)], & \text{if } r_m \neq 0, \\ 0, & \text{if } r_m = 0. \end{cases}$$

The numerical solution y_m at x_m satisfies the following relation

$$(30) \qquad \sum_{j=0}^{k} \alpha_{k-j} y_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} f(x_{m+k-j}, y_{m+k-j}) = 0, \quad 0 \le m \le N-k.$$

Subtracting (30) from (29), we get an error equation for r_m,

$$(31) \qquad \sum_{j=0}^{k} \alpha_{k-j} r_{m+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{k-j,m} g_{m+k-j} r_{m+k-j} = \varepsilon_{m+k}, \quad 0 \le m \le N-k.$$

Now we can apply Lemma 3 to the relation (31) with

$z_m = r_m$, $\Lambda = \varepsilon$, $N = (x_m - a)h^{-1}$, $A = \sum_{j=0}^{k} |\alpha_j|$,

$Z = 0$, (i.e., there is no initial round-off error),

$\beta_{k-j,m} = \hat{\beta}_{k-j,m} g_{m+k-j}$, $j = \delta_{t0}(1)k$,

$B = \sup_{m,h} \sum_{j=\delta_{t0}}^{k} |\hat{\beta}_{k-j,m}|$; $\quad \sum_{j=\delta_{t0}}^{k} |\beta_{k-j,m}| \le BL = B^*$, say.

Let $\beta = \sup_{m,h} |\hat{\beta}_{k,m}|$; then $|\beta_{k,m}| = |\hat{\beta}_{k,m} g_{m+k}| \le \beta L$.

Γ and γ are as defined in Lemma 2. Then proceeding as in the proof of Theorem 4, assuming that $h^2 < |\alpha_k|\, L^{-1}\beta^{-1}$,

$$|r_n| \le \varepsilon h^{-2}\Gamma^* \tfrac{1}{2}(x_n - a^*)^2 \exp\left((x_n - a^*)^2 \Gamma^* B^*\right).$$

Hence the proof.

2.8 Linear Multistep Method with Mildly Varying Coefficients

In this section we shall study a linear multistep method with mildly varying coefficients. The basic motivation comes from the work of Lambert [121] on multistep methods with mildly varying coefficients for first order initial value problems and the fact that our optimal multistep methods also fall in this category. We can interpret this situation as perturbations in α and β-coefficients of the usual method (2). Such a method for the initial value problem (1) in a neighbourhood of the initial point a, is given by

$$\sum_{j=0}^{k} \tilde{\alpha}_j(x_n)y_{n+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n)f_{n+j}, \tag{32}$$

with $\tilde{\alpha}_j(x) = \alpha_j+h^2a_j(x)$, and $\tilde{\beta}_j(x) = \beta_j+hb_j(x)$, where α_j, β_j are constants and $|a_j(x)| \le A_1$, and $|b_j(x)| \le B_1$, for all $x \in [a,b]$, $0 \le j \le k$, and A_1, B_1 are finite constants.

Let us define the linear difference operators L and M by

$$L[y(x);h] = \sum_{j=0}^{k} \alpha_j y(x+jh) - h^2 \sum_{j=0}^{k} \beta_j y''(x+jh),$$

and

$$M[y(x);x;h] = \sum_{j=0}^{k} a_j(x)y(x+jh) - h \sum_{j=0}^{k} b_j(x)y''(x+jh).$$

Then the linear difference operator associated with the perturbed method (32) is given by

$$\tilde{L}[y(x);x;h] = \sum_{j=0}^{k} (\alpha_j+h^2a_j(x))y(x+jh) - h^2 \sum_{j=0}^{k} (\beta_j+hb_j(x))y''(x+jh)$$

$$= \sum_{j=0}^{k} \alpha_j y(x+jh) - h^2 \sum_{j=0}^{k} \beta_j y''(x+jh) +$$

$$+ h^2\left(\sum_{j=0}^{k} a_j(x)y(x+jh) - h\sum_{j=0}^{k} b_j(x)y''(x+jh)\right)$$

$$= L[y(x);h] + h^2M[y(x);x;h].$$

L is the operator associated with the linear multistep method (2) with constant coefficients. Its order p is defined in Definition 1.

If M is applied to a sufficiently differentiable function y(x), then by Taylor's series expansion we have

$$M\,[y(x);x;h] = \sum_{j=0}^{k} a_j(x)y(x+jh) - h\sum_{j=0}^{k} b_j(x)y''(x+jh)$$

$$= D_0(x) + hD_1(x) + h^2D_2(x) + \ldots\ldots + h^rD_r(x) + \ldots\ldots,$$

where

$$D_0(x) = a_0(x)+a_1(x)+a_2(x)+\ldots\ldots+a_k(x),$$

$$D_1(x) = \{a_1(x)+2a_2(x)+3a_3(x)+\ldots\ldots+ka_k(x)\}y'(x)$$

$$- \{b_0(x)+b_1(x)+b_2(x)+\ldots\ldots+b_k(x)\}y''(x), \text{ and}$$

$$D_q(x) = \left(\frac{1}{q!}a_1(x)+\frac{2^q}{q!}a_2(x)+\ldots\ldots+\frac{k^q}{q!}a_k(x)\right)y^{(q)}(x)$$

$$- \left(\frac{1}{(q-1)!}b_1(x)+\frac{2^{q-1}}{(q-1)!}b_2(x)+\ldots\ldots+\frac{k^{q-1}}{(q-1)!}b_k(x)\right)y^{(q+1)}(x),$$

for $q = 2,3,\ldots$.

Since $\tilde{L}[y(x);x;h] = L[y(x);h] + h^2M[y(x);x;h]$, by Taylor's series expansion we get

$$\tilde{L}[y(x);x;h] = C_0y(x)+hC_1y'(x)+h^2C_2y''(x)+h^3C_3y^{(3)}(x)+\ldots\ldots$$

$$+h^2\left\{D_0(x) + hD_1(x) + h^2D_2(x) + \ldots\ldots\right\},$$

so that

$$\frac{1}{h^2}\tilde{L}[y(x);x;h] = \frac{1}{h^2}\left\{C_0y(x)+hC_1y'(x)+h^2C_2y''(x)+h^3C_3y^{(3)}(x)+\ldots\right\}$$

$$+\left\{D_0(x)+hD_1(x)+h^2D_2(x)+\ldots\ldots\right\}.$$

Since the left hand side is a difference approximation for the given differential equation, the right hand side should vanish as $h \to 0$. Thus we get the following definition.

Definition 3: The perturbed method (32) is consistent if $C_0 = C_1 = C_2 = 0$, and $D_0(x)=0$, for all $x \in [a,b]$.

Definition 4: The perturbed method (32) associated with the operator $\tilde{L}$ is said to be stable if the operator L is stable.

Theorem 7: A sufficient condition for the method (32) to be convergent is that it be stable and consistent.

Proof : Let the function f satisfy the conditions (i) and (ii) stated in section 1.1 and let η and η' be arbitrary constants. Let $y(x)$ be the solution of the initial value problem

$$y'' = f(x,y), \quad y(a) = \eta, \quad y'(a) = \eta'.$$

Let y_n, $(n=0,1,2,\ldots)$ be the solution of the difference scheme (32) defined by the starting values

$$y_\mu = \eta_\mu(h), \; \mu = 0,1,2,\ldots,k-1.$$

We set

$$\delta_1 = h\delta(h) = h\delta = \max_{0\le\mu\le k-1} |\eta_\mu(h) - y(a+\mu h)|,$$

$$\delta_2 = \max_{0 \le \mu \le k-1} \left| \frac{\eta_\mu(h)-\eta_0(h)}{\mu h} - y(a+\mu h) \right|,$$

and assume that $\lim_{h\to 0} \delta(h) = 0$, and $\lim_{h\to 0} \delta_2 = 0$. Then we have to show that for any x in [a,b]

$$\lim_{\substack{h\to 0 \\ x_n = x}} y_n = y(x).$$

The function $y''(x) = f(x,y)$ is continuous in [a,b]. Let us define the function

$$\chi(\varepsilon) = \max_{\substack{|x^* - x| < \varepsilon \\ x^*, x \in [a,b]}} |y''(x^*) - y''(x)|.$$

We know,

$$(33) \qquad y''(x_{m+\mu}) = y''(x_m) + \theta_\mu(\mu h), \quad \text{for } \mu = 0,1,..k,$$

where $|\theta_\mu| \le 1$. Again, since

$y(x_{m+\mu})=y(x_m) + \mu h\, y'(x_m) + \frac{(\mu h)^2}{2!} y''(\xi_\mu)$, where $x_m<\xi_\mu<x_{m+\mu}$, we get

$$(34) \qquad y(x_{m+\mu}) = y(x_m) + \mu h\, y'(x_m) + \frac{(\mu h)^2}{2!}\Big(y''(x_m) + \theta'_\mu\, \chi(\mu h)\Big),$$

where $|\theta'_\mu| \le 1$. Using (33) and (34), we get

$$L[y(x_m);h] = \sum_{j=0}^{k} \alpha_j y(x_m+jh) - h^2 \sum_{j=0}^{k} \beta_j y''(x_m+jh)$$

$$= (\alpha_0+\alpha_1+....+\alpha_k)y(x_m) + (\alpha_1+2\alpha_2 +....+k\alpha_k)hy'(x_m)$$

$$+ \left\{(\tfrac{1}{2!}\alpha_1+\tfrac{2^2}{2!}\alpha_2+....+\tfrac{k^2}{2!}\alpha_k) - (\beta_0+\beta_1+....+\beta_k)\right\}h^2y''(x_m)$$

$$+ \theta'\left\{\tfrac{1}{2!}|\alpha_1|+\tfrac{2^2}{2!}|\alpha_2|+....+\tfrac{k^2}{2!}|\alpha_k|\right\}h^2\chi(kh)$$

$$- \theta\left\{|\beta_0|+|\beta_1|+....+|\beta_k|\right\} h^2\chi(kh),$$

where $|\theta'| \le 1$ and $|\theta| \le 1$. By consistency of L we have,

$$|L\ [y(x_m);h]| \le Kh^2\chi(kh),$$

where $K = (\frac{1}{2!}|\alpha_1|+\frac{2^2}{2!}|\alpha_2|+...+\frac{k^2}{2!}|\alpha_k|)+(|\beta_0|+|\beta_1|+...+|\beta_k|)$.

Now if M is applied to a sufficiently differentiable function $y(x)$, then

$$\begin{aligned}M[y(x_m);x_m;h] &= \sum_{j=0}^{k} a_j(x_m)y(x_m+jh) - h^2\sum_{j=0}^{k} b_j(x_m)y''(x_m+jh)\\
&= (a_0(x_m)+a_1(x_m)+....+ a_k(x_m))y(x_m)\\
&\quad + (a_1(x_m)+2a_2(x_m)+....+ka_k(x_m))hy'(x_m)\\
&\quad + \left\{\frac{1}{2!}a_1(x_m)+\frac{2^2}{2!}a_2(x_m)+....+\frac{k^2}{2!}a_k(x_m)\right\}h^2y''(x_m)\\
&\quad + \phi'\left\{\frac{1}{2!}|a_1(x_m)|+\frac{2^2}{2!}|a_2(x_m)|+....+\frac{k^2}{2!}|a_k(x_m)|\right\}h^2\chi(kh)\\
&\quad - (b_0(x_m)+b_1(x_m)+....+b_k(x_m))hy''(x_m)\\
&\quad - \phi\left\{|b_0(x_m)|+|b_1(x_m)|+....+|b_k(x_m)|\right\}h\chi(kh),\end{aligned}$$

where $|\phi'| \le 1$ and $|\phi| \le 1$.

For all $x \in [a,b]$, we have the following :

(i) $|a_j(x_n)| \le A_1$, and $|b_j(x_n)| \le B_1$, $0 \le j \le k$;

(ii) by consistency, $D_0(x_m) = a_0(x_m)+a_1(x_m)+....+a_k(x_m) = 0$;

(iii) $|y''(x)| \le F_2$, where F_2 is a finite constant.

Since $y''(x) = f(x,y(x))$ is a continuous function of x on the closed

interval $[a,b]$, it is necessarily bounded on $[a,b]$, and

$$|y'(x)|=\left|\eta'+\int_a^x y''(x)dx\right| \le |\eta'|+\int_a^x |y''(x)|dx \le |\eta'|+F_2(b-a)=F_1, \quad \text{say.}$$

Using (i), (ii) and (iii) we have

$$|M\,[y(x_m);x_m;h]| \le A_1hF_1\,\frac{k(k+1)}{2} + A_1h^2F_2\,\frac{k(k+1)(2k+1)}{12}$$

$$+ A_1h^2\chi(kh)\,\frac{k(k+1)(2k+1)}{12} + B_1hF_2\,\frac{k(k+1)}{2} + B_1h\,\chi(kh)\,\frac{k(k+1)}{2}$$

$$= Gh, \text{ say,}$$

$$G = A_1F_1\,\frac{k(k+1)}{2} + A_1hF_2\,\frac{k(k+1)(2k+1)}{12} + A_1h\chi(kh)\,\frac{k(k+1)(2k+1)}{12}$$

$$+ B_1F_2\,\frac{k(k+1)}{2} + B_1\,\chi(kh)\,\frac{k(k+1)}{2} = O(1).$$

Then

$$|\tilde{L}[y(x_m);x_m;h]| \le |L\,[y(x_m);h]| + h^2\,|M\,[y(x_m);x_m;h]|$$

$$\le Kh^2\chi(kh) + Gh^3.$$

So, we can write

$$\tilde{L}\,[y(x_m);x_m;h] = \theta_m\left(Kh^2\chi(kh) + Gh^3\right), \quad \text{where } |\theta_m| \le 1, \quad \text{or,}$$

$$(33)\qquad \sum_{j=0}^{k}\tilde{\alpha}_j(x_m)y(x_{m+j}) - h^2\sum_{j=0}^{k}\tilde{\beta}_j(x_m)y''(x_{m+j}) = \theta_m\left(Kh^2\chi(kh) + Gh^3\right).$$

Let us define

(34) $e_m = y_m - y(x_m)$, the discretization error at the point x_m; and

$$(35)\qquad g_m = \begin{cases} [f(x_m,y_m) - f(x_m,y(x_m))]e_m^{-1}, & \text{if } e_m \ne 0, \\ 0, & \text{if } e_m = 0. \end{cases}$$

Subtracting (35) from the corresponding relation:

$$\sum_{j=0}^{k} \tilde{\alpha}_j(x_m)y_{m+j} - h^2\sum_{j=0}^{k} \tilde{\beta}_j(x_m)f_{m+j} = 0,$$

we get the following difference equation for e_m:

$$\sum_{j=0}^{k} \tilde{\alpha}_j(x_m)e_{m+j} - h^2\sum_{j=0}^{k} \tilde{\beta}_j(x_m)g_{m+j}e_{m+j} = \theta_m\left(Kh^2\chi(kh) + Gh^3\right).$$

Let us rewrite this equation as

$$(38)\quad \sum_{j=0}^{k}\alpha_j e_{m+j} - h^2\sum_{j=0}^{k}[\tilde{\beta}_j(x_m)g_{m+j} - a_j(x_m)]e_{m+j} = \theta_m\left(Kh^2\chi(kh)+Gh^3\right).$$

By Lipchitz condition, $|g_{m+j}| \le L$, $j = 0(1)k$, $m = 0,1,2,\ldots\ldots$. Now we can apply Lemma 3 to (38) with

$z_m = e_m$, $Z = h\delta(h)$, $\Lambda = Kh^2\chi(kh)+Gh^3$, $N = (x_m-a)h^{-1}$, $A = \sum_{j=0}^{k}|\alpha_j|$,

$B = \sum_{j=0}^{k}|\beta_j|$, $\beta_{jm} = \tilde{\beta}_j(x_m)g_{m+j}-a_j(x_m)$, $j = 0(1)k$,

$$\sum_{j=0}^{k}|\beta_{jm}| \le \sum_{j=0}^{k}\left\{\left(|\beta_j| + h|b_j(x_m)|\right)|g_{m+j}| + |a_j(x_m)|\right\}$$

$\le (B + h(k+1)B_1)L + (k+1)A_1$, and let

$$(39)\qquad B^* = [B + h(k+1)B_1]L + (k+1)A_1$$

$|\beta_{km}| \le (|\beta_k|+h|b_k(x_m)|)|g_{m+k}|+|a_k(x_m)| \le (|\beta_k|+hB_1)L+A_1 = \beta$, say,

and with Γ and γ as defined in Lemma 2. Let

$$(40)\qquad \Gamma^* = \frac{\Gamma}{1-h^2|\alpha_k^{-1}|\beta}, \quad\text{and}\quad a^* = a - \frac{h\gamma}{\Gamma}.$$

Then $N\Gamma + \gamma = (x_n-a^*)\Gamma h^{-1}$, and $\frac{1}{2}N^2\Gamma + N\gamma \le \frac{1}{2}(x_n-a^*)^2\Gamma h^{-2}$, and we

have

$$|e_n| \le \Gamma^*\Big((x_n-a^*)kA\delta + \frac{1}{2}(x_n-a^*)^2[K\chi(kh)+Gh]\Big)\exp\Big((x_n-a^*)^2\Gamma^*B^*\Big).$$

Since, $\delta \to 0$ as $h \to 0$, and $\chi(kh) \to 0$ as $h \to 0$, we have $e_n \to 0$ as $h \to 0$, $n \to \infty$. Hence the convergence.

2.9 A Bound for the Local Truncation Error

Lemma : Let

$$L\,[y(x);h] = \sum_{j=0}^{k}\alpha_j y(x+jh) - h^2\sum_{j=0}^{k}\beta_j y''(x+jh)$$

be the difference operator of order $p > 0$, corresponding to the usual method (2) and let

$$\tilde{L}\,[y(x);x;h] = \sum_{j=0}^{k}\tilde{\alpha}_j(x)y(x+jh) - h^2\sum_{j=0}^{k}\tilde{\beta}_j(x)y''(x+jh)$$

be the difference operator corresponding to the perturbed method (32). Let $y(x)$ possess a continuous derivative of order $\tilde{p}+2$ on the interval $[a,b]$, where $\tilde{p} = \min\{p,r+1\}$, r is an integer for which the forthcoming system of equations (41-i)-(41-ii) and (42-i)-(42-ii) hold, and set

$$\tilde{Y} = \max_{\substack{x\in[a,b]\\ 0\le i\le \tilde{p}+2}} |y^{(i)}(x)|.$$

Then $$|\ \tilde{L}[y(x);x;h]\ | \le h^{\tilde{p}+2}\,\tilde{G}\,\tilde{Y},$$

uniformly in x, $x+kh \in [a,b]$, where $\tilde{G}$ is a constant independent of y.

Proof: If $y(x)$ has continuous derivatives of order $n+2$ in $[a,b]$

and if x and $\bar{x}$ are in $[a,b]$, then by Taylor's theorem with the integral form of the remainder, we have

$$y(\bar{x}) = y(x) + (\bar{x}-x)y'(x) + \frac{(\bar{x}-x)^2}{2!}y''(x) + \ldots\ldots + \frac{(\bar{x}-x)^{n+1}}{(n+1)!}\,y^{(n+1)}(x)$$

$$+ \frac{1}{(n+1)!}\int_x^{\bar{x}} (\bar{x}-t)^{n+1}y^{(n+2)}(t)\,dt.$$

Now

$$\tilde{L}[y(x);x;h] = L[y(x);h] + h^2M[y(x);x;h].$$

Since $L\,[y(x);h]$ is of order $p > 0$, by Lemma 1, we have

$$|L\,[y(x);h]| \le h^{p+2}GY_1,$$

uniformly in x, $x+kh \in [a,b]$ where G is a constant independent of y and

$$Y_1 = \max_{x\in[a,b]} |y^{(p+2)}(x)|.$$

Now if $M[y(x);x;h]$ is applied to a function $y(x)$, having continuous derivative of order $r+1$, then

$$M\,[y(x);x;h] = \sum_{j=0}^{k} a_j(x)y(x+jh) - h^2\sum_{j=0}^{k} b_j(x)y''(x+jh)$$

$$=(a_0(x)+a_1(x)+\ldots.+a_k(x))y(x) +$$

$$+h\Big[\Big\{a_1(x)+2a_2(x)+\ldots.+ka_k(x)\Big\}y'(x)-\Big\{b_0(x)+b_1(x)+\ldots.+b_k(x)\Big\}y^{(2)}(x)\Big]$$

$$+ h^2\Big[\Big\{\frac{1}{2!}a_1(x)+\frac{2^2}{2!}a_2(x)+..+\frac{k^2}{2!}a_k(x)\Big\}y^{(2)}(x)$$

$$-\Big\{b_1(x)+2b_2(x)+..+kb_k(x)\Big\}y^{(3)}(x)\Big] +\ldots\ldots\ldots$$

$$+ h^r\Big[\Big\{\frac{1}{r!}a_1(x)+\frac{2^r}{r!}a_2(x)+\ldots.+\frac{k^r}{r!}\,a_k(x)\Big\}y^{(r)}(x)$$

$$- \left\{\frac{1}{(r-1)!}b_1(x)+\frac{2^{r-1}}{(r-1)!}b_2(x)+\dots+\frac{k^{r-1}}{(r-1)!}b_k(x)\right\}y^{(r+1)}(x)\Big]$$

$$+ h^{r+1}\left[\left\{\frac{1}{(r+1)!}a_1(x)+\frac{2^{r+1}}{(r+1)!}a_2(x)+\dots+\frac{k^{r+1}}{(r+1)!}a_k(x)\right\}\right]y^{(r+1)}(x)$$

$$+ \frac{1}{(r+1)!}\Big[a_1(x)\int_x^{x+h}(x+h-t)^{r+1}y^{(r+2)}(t)dt + a_2(x)\int_x^{x+2h}(x+2h-t)^{r+1}y^{(r+2)}(t)dt$$

$$+\dots\dots+ a_k(x)\int_x^{x+kh}(x+kh-t)^{r+1}y^{(r+2)}(t)dt\Big]$$

$$- \frac{h^2}{(r-1)!}\Big(b_1(x)\int_x^{x+h}(x+h-t)^{r-1}y^{(r+2)}(t)dt + b_2(x)\int_x^{x+2h}(x+2h-t)^{r-1}y^{(r+2)}(t)dt$$

$$+\dots\dots+ b_k(x)\int_x^{x+kh}(x+kh-t)^{r-1}y^{(r+2)}(t)dt\Big).$$

Let $a_i(x)$, $b_i(x)$; $i = 0(1)k$ satisfy the following equations:

(41-i) $\quad a_0(x) + a_1(x) +\dots+ a_k(x) = 0,$

(41-ii) $\quad \frac{1}{t!}a_1(x)+\frac{2^t}{t!}a_2(x) +\dots+ \frac{k^t}{t!}a_k(x) = 0, \quad t = 1(1)r+1,$ and

(42-i) $\quad b_0(x) + b_1(x) +\dots+ b_k(x) = 0,$

(42-ii) $\quad \frac{1}{t!}b_1(x)+\frac{2^t}{t!}b_2(x) +\dots+ \frac{k^t}{t!}b_k(x) = 0, \quad t = 1(1)r-1.$

Then, putting $t = x+sh$, we have

$$M[y(x);x;h] = \frac{h^{r+2}}{(r+1)!}\sum_{i=0}^{k}a_i(x)\int_0^i(i-s)^{r+1}y^{(r+2)}(x+sh)ds$$

$$- \frac{h^{r+1}}{(r-1)!}\sum_{i=0}^{k}b_i(x)\int_0^i(i-s)^{r-1}y^{(r+2)}(x+sh)ds.$$

Hence, $\qquad |M[y(x);x;h]| \le G_1h^{r+1}Y_1,$

where G_1 is independent of y, and $Y_1 = \max\limits_{x\in[a,b]} |y^{(r+2)}(x)|.$

Hence, $|\tilde{L}\ [y(x);x;h]| \le |L\ [y(x);h]| + h^2\ |M\ [y(x);x;h]|$

$$\le h^{p+2}GY + G_1 h^{r+3} Y_1 \le h^{\tilde{p}+2}\tilde{G}\tilde{Y} = O(h^{\tilde{p}+2}),$$

where $\tilde{p} = \min\{p, r+1\}$, $\tilde{Y} = \max\{Y, Y_1\}$ and $\tilde{G} = \max\{G, G_1\}$.

2.10 A Bound for the Discretization Error

Let us assume that the exact solution $y(x)$ has a continuous derivative of order $\tilde{p}+2$ for $x \in [a,b]$. Set

$$\tilde{Y} = \max_{a \le x \le b} |\ y^{(\tilde{p}+2)}(x)\ |, \tag{43}$$

where $\tilde{p} = \min(p, r+1)$; $p\ (>0)$ is the order of the usual operator $L\ [y(x);h]$ and r is a positive integer for which the systems of equations (41-i)-(41-ii) and (42-i)-(42-ii) hold good.

Instead of the difference equation (32) let the numerical solution y_n satisfy the following equation, at a point x_m

$$\sum_{j=0}^{k} \tilde{\alpha}_j(x_m) y_{m+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_m) f(x_{m+j}, y_{m+j}) + \theta_m K\ h^{q+2}, \quad 0 \le m \le N-k, \tag{44}$$

where $|\theta_m| \le 1$, and K, q are constants with $q > 0$. The term involving K stands for small error in the difference equation. Let us set the starting errors

$$|y_\mu - y(x_\mu)| \le h\delta(h), \quad \mu = 0(1)k-1 \tag{45}$$

<u>Theorem 8 :</u> Under the conditions (43), (44) and (45) if $h^2 < |\alpha_k \beta^{-1}|$, the discretization errors $e_n = y_n - y(x_n)$ satisfy the following relation, for $a \le x_n \le b$,

$$|e_n| \le \Gamma^*\left[(x_n-a^*)kA\delta(h) + \frac{1}{2}(x_n-a^*)^2\{Kh^q + \tilde{G}\ \tilde{Y}\ h^{\tilde{p}}\right]\exp\left\{(x_n-a^*)^2\Gamma^* B^*\right\},$$

where Γ^*, a^* are defined in (40), B^* is defined in (39). G^* is a constant depending only on $\tilde{L}\,[y(x);h]$, the difference operator associated with the optimal method (32) and L is the Lipchitz constant.

<u>Proof:</u> The exact solution y(x) satisfies the following relation at the point x_m

$$(46)\quad \sum_{j=0}^{k} \tilde{\alpha}_j(x_m)y(x_m+jh) = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_m)f(x_m+jh,y(x_m+jh))+\tilde{T}_m, \quad 0\le m\le N-k,$$

where $\tilde{T}_m$ is the local truncation error functional for the optimal method (32) at the point x_m. By Lemma 6, we have

$$|\ \tilde{T}_m\ | \le \tilde{G}\ \tilde{Y}\ h^{\tilde{p}+2}.$$

Hence, $\tilde{T}_m = \theta_{m1}\tilde{G}\ \tilde{Y}\ h^{\tilde{p}+2}$, where $|\ \theta_{m1}\ | \le 1$.

Let e_m and g_m be defined by (36) and (37). Subtracting (46) from (44), we get the error equation

$$(47)\quad \sum_{j=0}^{k} \tilde{\alpha}_j(x_m)e_{m+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_m)g_{m+j}e_{m+j} + \theta'_m\ (Kh^{q+2} + \tilde{G}\ \tilde{Y}\ h^{\tilde{p}+2}),$$

where $|\ \theta'_m\ | \le 1$. Now applying Lemma 3 to the difference equation (47), and proceeding as in Theorem 7, with the only exception that $\Lambda = Kh^{q+2}+\tilde{G}\tilde{Y}h^{\tilde{p}+2}$, we get for $h^2 < |\alpha_k\beta^{-1}|$,

$$|e_n| \le \Gamma^*\left[(x_n-a^*)kA\delta(h) + \frac{1}{2}(x_n-a^*)^2\{Kh^q + \tilde{G}\tilde{Y}h^{\tilde{p}}\}\right]\exp\left\{(x_n-a^*)^2\Gamma^* B^*\right\}.$$

<u>Remark:</u> If $\delta(h) = O(h^{\tilde{p}})$ and $q \ge \tilde{p}$, then $e_n = O(h^{\tilde{p}})$.

2.11 Propagation of Round-Off Error

Theorem 9: If $h^2 < |\alpha_k \beta^{-1}|$, the round-off error $r_n = \tilde{y}_n - y_n$ satisfies the following relation, for $a \le x_n \le b$,

$$|r_n| \le \varepsilon h^{-2} \Gamma^* \ \frac{1}{2}(x_n - a^*)^2 \exp\left((x_n - a^*)^2 \Gamma^* B^*\right), \quad 0 \le n \le N-k,$$

where Γ^* and a^* are defined in (40), B^* is defined in (39), L is the Lipchitz constant for the function f(x,y) and ε is a bound for the local round-off errors.

Proof: The numerical approximations $\{\tilde{y}_n\}$ to $\{y_n\}$ of the numerical method (32) satisfy the following equations,

$$(48) \qquad \sum_{j=0}^{k} \tilde{\alpha}_j(x_n)\tilde{y}_{n+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n) f(x_{n+j}, \tilde{y}_{n+j}) + \varepsilon_{n+k}, \qquad 0 \le n \le N-k,$$

where ε_n is the local round-off error which depends on the computational procedure and on the organization of the arithmetic unit of the computing equipment.

Let $r_n = \tilde{y}_n - y_n$ be the accumulated round-off error at a point x_n. Let $|\varepsilon_n| \le \varepsilon$, where ε is independent of n. Let

$$r_m = \begin{cases} r_m^{-1} \, [f(x_m, \tilde{y}_m) - f(x_m, y_m)], & \text{if } r_m \ne 0, \\ 0, & \text{if } r_m = 0. \end{cases}$$

Subtracting (46) from the corresponding relation:

$$\sum_{j=0}^{k} \tilde{\alpha}_j(x_n) y_{n+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n) f(x_{n+j}, y_{n+j}),$$

we get the following equation:

$$\sum_{j=0}^{k}\tilde{\alpha}_j(x_n)r_{n+j} = h^2\sum_{j=0}^{k}\tilde{\beta}_j(x_n)g_{n+j}\, r_{n+j} + \varepsilon_{n+k},$$

Rewriting this equation in the form:

$$\sum_{j=0}^{k}\alpha_j r_{n+j} = h^2\sum_{j=0}^{k}\{\tilde{\beta}_j(x_n)g_{n+j} - a_j(x_n)\}r_{n+j} + \varepsilon_{n+k},$$

and applying Lemma 3 to this equation, with $z_m = r_m$, $Z = 0$ (i.e. there is no initial round-off error), $\Lambda = \varepsilon$, $N = (x_m - a)h^{-1}$,

$\beta_{jm} = \tilde{\beta}_j(x_m)g_{m+j} - a_j(x_m) = \{\beta_j + hb_j(x_m)\}g_{m+j} - a_j(x_m)$, $j = 0(1)k$,

$A = \sum_{j=0}^{k}|\alpha_j|$, $B = \sum_{j=0}^{k}|\beta_j|$, we get, as in the proof of Theorem 7,

$$\sum_{j=0}^{k}|\beta_{jm}| \le (B + h(k+1)B_1)L + (k+1)A_1 = B^*, \text{ say,}$$

$|\beta_{km}| \le (|\beta_k| + hB_1)L + A_1 = \beta$, say, and $\Gamma^* = \dfrac{\Gamma}{1 - h^2L|\alpha_k^{-1}|\beta}$, $a^* = a - \dfrac{h\gamma}{\Gamma}$.

Thus assuming that $h^2 < |\alpha_k|\,\beta^{-1}$, we have

$$|r_n| \le \varepsilon h^{-2}\Gamma^*\,\frac{1}{2}(x_n - a^*)^2\exp\left((x_n - a^*)^2\Gamma^* B^*\right).$$ Hence the proof.

2.12 Stability Analysis of Linear Multistep Methods With Varying Coefficients

Let the equation (32) be a linear multistep method with mildl varying coefficients corresponding to a consistent and stab. linear multistep method (2) with constant coefficients.

Let at a point x_n the exact solution $y(x)$ of the differenti equation satisfy

(49) $$\sum_{j=0}^{k} \tilde{\alpha}_j(x_n)y(x_{n+j}) = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n)f(x_{n+j},y(x_{n+j})) + T_n,$$

where T_n is the local truncation error at x_n. If $\{y_n\}$ denotes the computed solution of the difference equation (49), then

(50) $$\sum_{j=0}^{k} \tilde{\alpha}_j(x_n)y_{n+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n)f_{n+j} + R_n,$$

where R_n is the local round off error at x_n. Subtracting (50) from (49), and applying mean value theorem we get the following equation for the discretisation error $e_n = y(x_n) - y_n$:

(51) $$\sum_{j=0}^{k} \tilde{\alpha}_j(x_n)e_{n+j} = h^2 \sum_{j=0}^{k} \tilde{\beta}_j(x_n)\frac{\partial f}{\partial y}(x_{n+j},\xi_{n+j})e_{n+j} + E_n,$$

where $\xi_{n+j} \in (y_{n+j}, y(x_{n+j}))$ and $E_n = T_n - R_n$.

Let us assume that $\frac{\partial f}{\partial y}(x_{n+j},\xi_{n+j}) = -q(x_{n+j})$, $j = 0(1)k$, i.e., the function f is linear in y. Then the error equation (51) becomes,

$$\sum_{j=0}^{k} \left\{\tilde{\alpha}_j(x_n) + h^2 q(x_{n+j})\tilde{\beta}_j(x_n)\right\} e_{n+j} = E_n,$$

or, $$\sum_{j=0}^{k} \left\{\alpha_j + h^2\left(a_j(x_n) + q(x_{n+j})[\beta_j + h\, b_j(x_n)]\right\}\right. e_{n+j} = E_n,$$

or,

(52) $$\sum_{j=0}^{k} \alpha_j e_{n+j} = E_n - h^2 \sum_{j=0}^{k} \phi_j(n)e_{n+j},$$

where $\phi_j(n) = a_j(x_n) + q(x_{n+j})[\beta_j + h\, b_j(x_n)]$, $j = 0(1)k$. Without loss of generality, we can assume that $\alpha_k = 1$.

Equation (52) is a linear difference equation with constant coefficients with an inhomogeneous term represented by the whole of right hand side. The complete solution of such an equation may be expressed as the sum of the complementary function and a particular

solution; moreover, the latter may be represented as the convolution of the inhomogeneous term with the particular solution of the reduced equation (53), given below.

Let $\{\eta_n\}$ be the complete solution of the reduced equation,

$$(53) \qquad \sum_{j=0}^{k} \alpha_j e_{n+j} = 0.$$

The characteristic equation associated with the difference equation (53) is given by

$$\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j = 0.$$

Assume that the usual linear multistep method (2) is consistent and stable. By its consistency, we have

$$\rho(1) = 0, \ \rho'(1) = 0, \ \rho''(1) = 2\sigma(1) \neq 0,$$

i.e., $\zeta = 1$ is a double root of the equation $\rho(\zeta) = 0$. Let this root be $\zeta = \zeta_1$. If the other roots of $\rho(\zeta) = 0$ are distinct, say ζ_μ, $3 \le \mu \le k$, then

$$\eta_n = (A_1 + nA_2)\zeta_1^n + \sum_{p=3}^{k} A_p \zeta_p^n = (A_1 + nA_2) + \sum_{p=3}^{k} A_p \zeta_p^n .$$

In general, if the distinct roots, other than 1, are ζ_μ, $3 \le \mu \le \tilde{k}$, say, let the root ζ_μ, of $\rho(\zeta) = 0$, have the multiplicity p_μ, $3 \le \mu \le \tilde{k}$, so that $\sum_{\mu} p_\mu = k-2$. Then

$$(54) \quad \eta_n = (A_1 + nA_2) + \sum_{3 \le \mu \le \tilde{k}} \left\{ B_{\mu,0} + nB_{\mu,1} + n(n-1)B_{\mu,2} + \ldots + n(n-1)\ldots(n-p_\mu+2)B_{\mu,p_\mu-1} \right\} \zeta_\mu^n$$

where the coefficients:

$$A_1,\ A_2,\ \left\{B_{\mu,i},\ i = 0(1)p_\mu - 1,\ 3 \le \mu \le \tilde{k}\right\}$$

are to be determined through the initial values $e_0, e_1, e_2, \ldots, e_{k-1}$; where the particular solution $\{z_n\}$ of equation (53) satisfies the initial conditions $z_0 = z_1 = \ldots = z_{k-2} = 0$, $z_{k-1} = 1$, we have

$$(55) \qquad e_n = \eta_n + \sum_{t=1}^{n} z_{n-t} d_t = \eta_n + \sum_{t=1}^{n-1} z_{n-t} d_t,$$

where

$$(56) \qquad d_t = E_{t-1} - h^2 \sum_{j=0}^{k} \phi_j(t-1) e_{t+j-1}, \quad t \ge 0.$$

Following Lambert [121], let us define

$$(57) \qquad d_t^* = E_{t-1} - h^2 \sum_{j=0}^{k} \phi_j(t-1) \eta_{t+j-1}.$$

Then by (56) and (57), we have

$$\begin{aligned} d_t^* - d_t &= h^2 \sum_{j=0}^{k} \phi_j(t-1) \left\{ e_{t+j-1} - \eta_{t+j-1} \right\} \\ &= h^2 \sum_{j=0}^{k} \phi_j(t-1) \left\{ \eta_{t+j-1} + \sum_{s=1}^{t+j-2} z_{t+j-1-s} d_s - \eta_{t+j-1} \right\} \\ &= h^2 \sum_{j=0}^{k} \phi_j(t-1) \left\{ \sum_{s=1}^{t+j-2} z_{t+j-1-s} d_s \right\} \\ &= h^2 \sum_{s=1}^{t+k-2} \left\{ \sum_{j=0}^{k} \phi_j(t-1) z_{t+j-1-s} \right\} d_s. \end{aligned}$$

We take z_n to be zero, when n is a negative integer. From the definition of z_n, we see that the expression in braces in the last expression vanishes when $t < s$, and hence we may write for $k \ge 2$,

$$(58) \qquad d_t^* = d_t + h^2 \sum_{s=1}^{t} \Phi_{ts}\, d_s, \qquad t = 1, 2, \ldots\ldots, T,$$

where $\Phi_{ts} = \sum_{j=0}^{k} \phi_j(t-1) z_{t+j-1-s}$ and $T \geq 1$. For any fixed $T \leq N$, let us define the vectors

$$d = (d_1,\ d_2, \ldots\ldots, d_T)^T, \quad \text{and} \quad d^* = (d_1^*,\ d_2^*, \ldots\ldots, d_T^*)^T.$$

Since $\Phi_{ts} = 0$ when $s > t$, Φ is a lower triangular matrix. Then

$$d^* = d + h^2\Phi d = (I + h^2\Phi)d.$$

Since z_n is an η_n, where the constants in η_n are to be determined by the conditions $z_0 = z_1 = \ldots = z_{k-2} = 0$, $z_{k-1} = 1$, and since the usual method is stable, $z_n = O(n)$. Again from (53), $\phi_j(t-1) = O(1)$.

So, $\quad \Phi_{ts} = O(t)$. But $\Phi_{tt} = \sum_{j=0}^{k} \phi_j(t-1) z_{j-1} = O(1)$.

Hence for all sufficiently small h, $(I + h^2\Phi)^{-1}$ exists and

$$d = (I + h^2\Phi)^{-1} d^*,$$

or,

(59) $$d_t = \sum_{s=1}^{t} \psi_{ts} d_s^*, \qquad t = 1,2,\ldots,T.$$

Φ being a lower triangular matrix, $\Psi = (I + h^2\Phi)^{-1} = (\psi_{ts})$ is also so. Hence $\psi_{ts} = 0$, when $s > t$, $t = 1,2,\ldots,T$. So, the solution (55) can be written as

(60) $$e_n = \eta_n + \sum_{t=1}^{n-1} z_{n-t} \left\{ \sum_{s=1}^{t} \psi_{ts} d_s^* \right\}.$$

Now from (57) and (54), we have

$$d_t^* = E_{t-1} - h^2 \sum_{j=0}^{k} \phi_j(t-1) \Big[A_1 + (t+j-1)A_2 + \sum_{\mu} \Big\{ B_{\mu,0} + (t+j-1)B_{\mu,1} +$$

$$(t+j-1)(t+j-2)B_{\mu,2} + \ldots + (t+j-1)(t+j-2)\ldots(t+j+1-p_\mu)B_{\mu,p_\mu-1} \Big\} \zeta_\mu^{t+j-1} \Big],$$

or, $$d_t^* = E_{t-1} - h^2\left[A_1F_1(t-1) + A_2F_2(t-1) + \sum_{\mu} \zeta_\mu^{t-1}F_\mu(t-1)\right],$$

where

(61-i) $$F_1(t-1) = \sum_{j=0}^{k}\phi_j(t-1), \qquad F_2(t-1) = \sum_{j=0}^{k}(t+j-1)\phi_j(t-1),$$

and for $3 \le \mu \le \tilde{k}$,

(61-ii) $$\begin{aligned} F_\mu(t-1) &= B_{\mu,0}\sum_{j=0}^{k}\phi_j(t-1)\zeta_\mu^j + B_{\mu,1}\sum_{j=0}^{k}(t+j-1)\phi_j(t-1)\zeta_\mu^j + \\ &\quad + B_{\mu,2}\sum_{j=0}^{k}(t+j-1)(t+j-2)\phi_j(t-1)\zeta_\mu^j + \ldots\ldots\ldots + \\ &\quad + B_{\mu,p_\mu-1}\sum_{j=0}^{k}(t+j-1)(t+j-2)\ldots(t+j-p_\mu+1)\phi_j(t-1)\zeta_\mu^j \\ &= B_{\mu,0}F_{\mu,0}(t-1)+B_{\mu,1}F_{\mu,1}(t-1)+\ldots+B_{\mu,p_\mu-1}F_{\mu,p_\mu-1}(t-1), \end{aligned}$$

where $F_{\mu,0}(t-1) = \sum_{j=0}^{k}\phi_j(t-1)\zeta_\mu^j$, and

$$F_{\mu,i}(t-1) = \sum_{j=0}^{k}(t+j-1)(t+j-2)\ldots(t+j-i)\phi_j(t-1)\zeta_\mu^j, \quad i=1(1)p_\mu-1.$$

Then

$$\begin{aligned} e_n &= (A_1 + nA_2) \\ &+ \sum_{\mu}\left\{B_{\mu,0}+ nB_{\mu,1}+ n(n-1)B_{\mu,2}+\ldots+n(n-1)\ldots(n-p_\mu+2)B_{\mu,p_\mu-1}\right\}\zeta_\mu^n \\ &+\sum_{t=1}^{n-1} z_{n-t}\left[\sum_{s=1}^{t}\psi_{ts}\left\{E_{s-1} - h^2\left(A_1F_1(s-1) + A_2F_2(s-1) + \sum_{\mu}\zeta_\mu^{s-1}F_\mu(s-1)\right)\right\}\right], \end{aligned}$$

or,

(62) $$e_n= A_1\left(1-h^2\sum_{t=1}^{n-1} z_{n-t}\sum_{s=1}^{t}\psi_{ts}F_1(s-1)\right)+A_2\left(n-h^2\sum_{t=1}^{n-1} z_{n-t}\sum_{s=1}^{t}\psi_{ts}F_2(s-1)\right)$$

$$+ \sum_{\mu} \left[B_{\mu,0}\left\{\zeta_\mu^n - h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1} F_{\mu,0}(s-1)\right\}\right.$$

$$+ B_{\mu,1}\left\{n\zeta_\mu^n - h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1} F_{\mu,1}(s-1)\right\} + \ldots .$$

$$\left. + B_{\mu,p_\mu-1}\left\{n(n-1)\ldots(n-p_\mu+2)\zeta_\mu^n - h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1} F_{\mu,p_\mu-1}(s-1)\right\}\right]$$

$$+ \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} E_{s-1},$$

or,

(63) $$e_n = A_1[1 + P_1(n)] + A_2[n + P_2(n)] + \sum_{\mu} \left[B_{\mu,0}\left\{\zeta_\mu^n + P_{\mu,0}(n)\right\} + \right.$$

$$B_{\mu,1}\left\{n\zeta_\mu^n + P_{\mu,1}(n)\right\} + \ldots + B_{\mu,p_\mu-1}\left\{n(n-1)\ldots(n-p_\mu+2)\zeta_\mu^n + P_{\mu,p_\mu-1}(n)\right\}$$

$$+ \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} E_{s-1},$$

where

(64) $$\begin{cases} P_j(n) = -h^2 \displaystyle\sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} F_j(s-1), \quad j = 1,2 \\ \\ P_{\mu,i}(n) = -h^2 \displaystyle\sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} \zeta_\mu^{s-1} F_{\mu,i}(s-1), \quad i=0(1)p_\mu-1, \ 3 \le \mu \le \tilde{k}. \end{cases}$$

Comparing (62) and (63), we see that

$$P_1(n),\ P_2(n),\ \left\{P_{\mu,0}(n),\ P_{\mu,1}(n), \ldots, P_{\mu,p_\mu-1}(n);\ 3 \le \mu \le \tilde{k}\right\}$$

may be interpreted as the perturbation corresponding to the fundamental solutions:

$$\zeta_1^n\ (=1),\ n\zeta_1^n\ (=n),\ \left\{\zeta_\mu^n,\ n\zeta_\mu^n, \ldots, n(n-1)(n-p_\mu+2)\zeta_\mu^n,\ 3 \le \mu \le \tilde{k}\right\}$$

of the equation

$$\sum_{j=0}^{k} \alpha_j e_{n+j} = 0.$$

Now we shall find the order of magnitude of ψ_{ts}. For this, $\psi_{tt} = (1+h^2\Phi_{tt})^{-1} = O(1)$, since $\Phi_{tt} = O(1)$. Assume that $\psi_{ts} = O(h^2)$, for $s < t$, $t = 2,3,\ldots q$; for convenience of notation, identifying $\Phi_{t,s}$ with Φ_{ts} and $\psi_{t,s}$ with ψ_{ts}, by (58) and (59), we get

$$d^*_{q+1} = d_{q+1} + h^2 \sum_{s=1}^{q+1} \Phi_{q+1,s} d_s,$$

or, $$d^*_{q+1} = (1 + h^2\Phi_{q+1,q+1})d_{q+1} + h^2 \sum_{s=1}^{q} \Phi_{q+1,s}\left(\sum_{u=1}^{s} \psi_{su} d^*_u\right),$$

or, $$d^*_{q+1} = (1 + h^2\Phi_{q+1,q+1})d_{q+1} + h^2 \sum_{u=1}^{q}\left\{\sum_{s=u}^{q} \Phi_{q+1,s}\psi_{su}\right\} d^*_u,$$

or,

$$d_{q+1} = \frac{1}{(1+h^2\Phi_{q+1,q=1})} d^*_{q+1} - \frac{h^2}{(1+h^2\Phi_{q+1,q+1})} \sum_{u=1}^{q}\left\{\sum_{s=u}^{q} \Phi_{q+1,s}\psi_{su}\right\} d^*_u.$$

Again from (59), we get

$$d_{q+1} = \sum_{s=1}^{q+1} \psi_{q+1,s} d^*_s = \psi_{q+1,q+1} d^*_{q+1} + \sum_{s=1}^{q} \psi_{q+1,s} d^*_s.$$

Comparing these two relations for d_{q+1}, we get

$$(65) \qquad \begin{cases} \psi_{q+1,q+1} = \dfrac{1}{(1+h^2\Phi_{q+1,q=1})}, \\[2ex] \psi_{q+1,u} = \dfrac{-\,h^2}{(1+h^2\Phi_{q+1,q+1})} \displaystyle\sum_{s=u}^{q} \Phi_{q+1,s}\psi_{su}, \quad u = 1(1)q. \end{cases}$$

Now, since $q \le n$, and $\Phi_{q+1,s} = O(n)$, and by hypothesis, $\psi_{su} = O(h^2)$, for $u < s \le q$

$$\psi_{q+1,u} = O(h^2), \quad u = 1(1)q.$$

To complete the induction, we note that indeed

$$\psi_{21} = - h^2\Phi_{21}(1 + h^2\Phi_{11})^{-1}(1 + h^2\Phi_{22})^{-1} = O(h^2).$$

Hence we conclude that

$$\psi_{ts} = O(h^2), \text{ as } h \to 0, \quad \text{for } s < t.$$

Since by the stability of the usual method (2), we know

$$|\zeta_\mu| \le 1, \quad 1 \le \mu \le k,$$

and $\psi_{ts} = O(h^2)$, for $s < t$, and $t \le n$, from (61-i) and (61-ii), we observe that:

if $F_j(s-1)=O(h)$, $j=1,2$ and $F_{\mu,i}(s-1)=O(h)$, $i= 0(1)p_\mu-1$, for all s

then $\sum_{s=1}^{t} \psi_{ts}F_j(s-1) = O(h)$, for $j = 1,2$, and

$$\sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1}F_{\mu,i}(s-1) = O(h), \; i = 0(1)p_\mu-1, \text{ for all } s.$$

Since $z_n = O(n)$, and $t \le n$, from (64), we have

$$P_j(n) = - h^2 \sum_{t=1}^{n-1} z_{n-t}\left(\sum_{s=1}^{t} \psi_{ts}F_j(s-1)\right) = O(h), \quad \text{for } j = 1,2;$$

and

$$P_{\mu,i}(n) = - h^2 \sum_{t=1}^{n-1} z_{n-t}\left(\sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1}F_{\mu,i}(s-1)\right) = O(h), \; i = 0(1)p_\mu-1,$$

$$3 \le \mu \le \tilde{k}.$$

Now we shall study some stability criteria of the multistep method (32) with mildly varying coefficients. For solving an

initial value problem (1), according to a usual method, the computed numerical solution satisfies at a point x_n:

(67) $$\sum_{j=0}^{k} \alpha_j y_{n+j} = h^2 \sum_{j=0}^{k} \beta_j f_{n+j} + R_n,$$

where R_n is the round off error at x_n. The true solution satisfies

(68) $$\sum_{j=0}^{k} \alpha_j y(x_{n+j}) = h^2 \sum_{j=0}^{k} \beta_j f(x_{n+j}, y(x_{n+j})) + T_n,$$

where T_n is the local truncation error at x_n. Subtracting (67) from (68), and applying Mean Value Theorem, we get the equation for the discretisation error $e_n = y(x_n) - y_n$,

$$\sum_{j=0}^{k} \alpha_j e_{n+j} = h^2 \sum_{j=0}^{k} \beta_j \frac{\partial f}{\partial y} (x_{n+j}, \xi_{n+j}) e_{n+j} + E_n,$$

where $\xi_{n+j} \in (y_{n+j}, y(x_{n+j}))$ and $E_n = T_n - R_n$. Assume that $E_n = E$, a constant and $\frac{\partial f}{\partial y}(x,y) = -q$, a constant, then the above error equation becomes

(69) $$\sum_{j=0}^{k} (\alpha_j + h^2 q \beta_j) e_{n+j} = E.$$

Let $\zeta_{\mu h}$, $\mu = 1(1)k$ be the k distinct roots of the polynomial

$$\sum_{j=0}^{k} (\alpha_j + h^2 q \beta_j) \zeta^j = 0,$$

or, $$\rho(\zeta) + h^2 q \sigma(\zeta) = 0,$$

where $\rho(\zeta) = \sum_{j=0}^{k} \alpha_j \zeta^j$ and $\sigma(\zeta) = \sum_{j=0}^{k} \beta_j \zeta^j$;

then the solution of the error equation (69) is

(70) $$e_n = \sum_{\mu=1}^{k} A_\mu \zeta_{\mu h}^n + \text{(particular solution involving E)}.$$

Let ζ_μ, $\mu = 1(1)k$, be the k roots of the equations $\rho(\zeta) = 0$. Then by the stability of the usual method (2), $|\zeta_\mu| \le 1$, $\mu = 1(1)k$. By its consistency, $\rho(1) = 0$, $\rho'(1) = 0$, So, $\zeta = 1$ is a double root of the equation $\rho(\zeta) = 0$.

Definition 3: We define a multistep method of the form (2) to be weakly stable if there is no other double root of the equation $\rho(\zeta) = 0$, on the unit circle, except $\zeta = 1$.

Now for a weakly stable usual method (2), $\zeta_{\mu h}$, the root of the equation $\rho(\zeta) + h^2\sigma(\zeta) = 0$, corresponding to a simple root ζ_μ of the equation $\rho(\zeta) = 0$ on the unit circle, may lie outside the unit circle, and its contribution $\zeta_{\mu h}^n$ to the error given by (70) will produce an uncontrolled growth.

Now let us consider the situation if we use the perturbed difference method (32) instead of the usual method (2) for the numerical solution of the initial value problem (1). Suppose the usual method (2) is weakly stable, and let ζ_μ be a simple root of the equation $\rho(\zeta) = 0$ on the unit circle. In this situation if we can choose $a_j(x)$ and $b_j(x)$ in such a way that

$$F_{\mu,0}(s-1) = O(h) \text{ for all } s, \quad 3 \le \mu \le \tilde{k},$$

then the perturbation $P_{\mu,0}(n)$ of the corresponding fundamental solution ζ_μ^n of the equation :

$$\sum_{j=0}^{k} \alpha_j e_{n+j} = 0,$$

will remain under control and will be of $O(h)$.

Let us consider other stability criteria of the method (32). The solution of an initial value problem of the form

$$y'' = \lambda y, \quad y(t_0) = y_0, \; y'(t_0) = y_0',$$

is given by

$$y(x) = C_1 \exp\{\sqrt{\lambda} x\} + C_2 \exp\{-\sqrt{\lambda} x\},$$

where $C_1 = \dfrac{(y_0\sqrt{\lambda} + y_0')\exp\{-\sqrt{\lambda} t_0\}}{2\sqrt{\lambda}}$, $\quad C_2 = \dfrac{(y_0 - y_0')\exp\{\sqrt{\lambda} t_0\}}{2\sqrt{\lambda}}$.

If the initial conditions $y(t_0)$ and $y'(t_0)$ are so chosen that $C_2 = 0$, e.g., if $y_0 = y_0'$, then $y(x) = C_1 \exp\{\sqrt{\lambda} x\}$, and $y(x) \to 0$, for all x, for the points of the set $\{\lambda: \mathrm{Re}\sqrt{\lambda} < 0\}$.

Now we define A_1 stability as follows.

Definition 4 : A linear multistep method of the form (2) applied to an initial value problem of the form

$$(71) \qquad y'' = \lambda y, \quad y(t_0) = y'(t_0) = y_0,$$

where λ is a complex constant such that $\mathrm{Re}\,\{\sqrt{\lambda}\} < 0$, is called A_1 stable if all the solutions of this method tend to zero, as $h \longrightarrow 0$, $n \longrightarrow \infty$, for the critical regeion, $x_n = o(h^{-1/2})$.
(Note that asking $y_n \longrightarrow 0$, for general $x_n \longrightarrow \infty$, is too restrictive a condition.)

Now let us apply a perturbed linear multistep method of the form (32), where $\frac{\partial f}{\partial y} = -q(x_n) = \lambda$, a complex constant, to an initial value of the form (71) with $\mathrm{Re}\,\{\sqrt{\lambda}\} < 0$, then the true solution of the initial value problem (71), $y(x) \to 0$, for all $x \longrightarrow \infty$.

The discretisation error, $e_n = y_n - y(x_n)$, at the point x_n is given by the expression (64) or (65) where $\frac{\partial f}{\partial y} = - q(x_n)$ is being replaced by λ in the expressions for $\phi_j(s-1)$, that is,

$$\phi_j(s-1) = a_j(x_{s-1}) - h\lambda\{\beta_j + hb_j(x_{s-1})\}.$$

Then $F_j(s-1)$, $j = 1,2$ and $F_{\mu,i}(s-1)$, $i = 0(1)p_\mu-1$, given by (61-i) and (61-ii) are with this definition of $\phi_j(s-1)$.

The k constants

$$A_1,\ A_2,\ \left\{B_{\mu,i},\ i = 0(1)p_\mu-1,\ 3 \le \mu \le \tilde{k}\right\}$$

of the error solution (63) are to be determined through the initial values of errors $e_0, e_1, \ldots, e_{k-1}$, using some one-step method. If

(72) $$e_i = y_i - y(x_i) = O(h^2), \quad i = 0(1)k-1,$$

that is, the initial values y_i, $i = 0(1)k-1$, are accurate of $O(h^2)$ to the actual solution $y(x_i)$, $i = 0(1)k-1$, then the above constants will have the order of magnitude of $O(h^2)$.

By stability of the usual method (2), we have $|\zeta_\mu| \le 1$. Since $\psi_{ts} = O(h^2)$, for $s < t$, and and $\psi_{tt} = O(1)$, $t \le n$, we observe that if

(73-i) $$F_j(s-1) = O(1), \quad j = 1,2, \quad \text{and}$$

(73-ii) $$F_{\mu,i}(s-1) = O(1), \quad i = 0(1)p_\mu-1, \text{ for all } s,$$

then $$\sum_{s=1}^{t} \psi_{ts}F_j(s-1) = O(1), \quad \text{for } j = 1,2,$$

and $$\sum_{s=1}^{t} \psi_{ts}\zeta_\mu^{s-1}F_{\mu,i}(s-1) = O(1),\ i = 0(1)p_\mu-1, \text{ for all } s.$$

Since $z_n = O(n)$ and $t \le n$, assuming that $nh = o(h^{-1/2})$,

$$P_j(n) = -h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts}F_j(s-1) = o(h^{-1}), \quad \text{for } j = 1,2, \quad \text{and}$$

$$P_{\mu,i}(n) = -h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} \zeta_\mu^{s-1} F_{\mu,i}(s-1) = o(h^{-1}),\ i = 0(1)p_\mu - 1,$$

$$\text{for } 3 \le \mu \le \tilde{k}.$$

We know that due to the local truncation error for the method at x_n is

$$T_n = O(h^3), \text{ if } r \ge 2, \quad \text{where } r \text{ is defined as earlier.}$$

If the round-off error R_n of the method satisfies the following relation:

(74) $$R_n = O(h^3),$$

then $$E_n = T_n - R_n = O(h^3).$$

Since $\psi_{ts} = O(h^2)$, for $s < t$, and $t \le n$, and $z_n = O(n)$, and $\psi_{tt} = O(1)$, and $nh = o(h^{-1/2})$, we have

$$\sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} E_{s-1} = o(1).$$

Then from (63), we see that under the assumptions (72), (73-i), (73-ii) and (74) $e_n \longrightarrow 0$ as $h \longrightarrow 0$, in the critical region $x_n = o(h^{-1/2})$.

Let us assume that the given usual method (2) is A_1-stable. Then under the assumptions (72), (73-i), (73-ii) and (74), the numerical solution $y_n = y(x_n)+e_n$ of the perturbed linear multistep method (32) applied to a model initial value problem (71) with Re $\{\sqrt{\lambda}\} < 0$, tends to zero, as $h \longrightarrow 0$, $n \longrightarrow \infty$ and $x_n = o(h^{-1/2})$, provided $r \ge 2$. Hence the perturbed linear multistep method (32) is A_1-stable under the assumptions (72), (73-i), (73-ii) and (74) in the critical region $x_n = o(h^{-1/2})$, provided $r \ge 2$.

Now we are defining A_2 stability as follows.

Definition 5 : A linear multistep method (2) when applied to an initial value problem of the form (71), where λ is a complex constant, is called A_2-stable if all the solutions of this method are bounded as $h \longrightarrow 0$, $n \longrightarrow \infty$, in the larger critical region $x_n = O(h^{-1/2})$, provided $r \geq 2$.

Suppose, the perturbed linear multistep method (32) is applied to a model initial value problem of the form (71), then the solution of its error equation (53), is given by (63), where $\frac{\partial f}{\partial y} = -q(x_n)$, is being replaced by λ in the expressions for $F_1(s-1)$, $F_2(s-1)$ and $F_{\mu,i}(s-1)$, $i = 0(1)p_\mu-1$, $3 \leq \mu \leq \tilde{k}$, given by (61-i) and (61-ii). If

(75) $$e_i = y_i - y(x_i) = O(h^2), \quad i = 0(1)k-1,$$

then the constants A_1, A_2, $\left\{B_{\mu,i},\ i = 0(1)p_\mu-1,\ 3 \leq \mu \leq \tilde{k}\right\}$ in the expression (63) for e_n is of the order of magnitude of $O(h^2)$. If

(76-i) $$F_j(s-1) = O(1),\ j = 1,2, \quad \text{and}$$

(76-ii) $$F_{\mu,i}(s-1) = O(1),\ i = 0(1)p_\mu-1, \text{ for all } s,$$

then since $\psi_{ts} = O(h)$, for $s < t$, $z_n = O(n)$, and $t \leq n$,

$$P_j(n) = -h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} F_j(s-1) = O(h^{-1}), \quad \text{for } j = 1,2, \quad \text{and}$$

$$P_{\mu,i}(n) = -h^2 \sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} \zeta_\mu^{s-1} F_{\mu,i}(s-1) = O(h^{-1}), \quad i = 0(1)p_\mu-1,$$

$$3 \leq \mu \leq \tilde{k}.$$

Suppose the local truncation error for the method is

$T_n = O(h^3)$, provided $r \geq 2$, where r is defined earlier.

If the round-off error of the method is

(77) $$R_n = O(h^3),$$

then $E_n = T_n - R_n = O(h^3)$. Since $\psi_{ts} = O(h^2)$, for $s < t$, and $t \leq n$, and $\psi_{tt} = O(1)$, $z_n = O(n)$, we have

$$\sum_{t=1}^{n-1} z_{n-t} \sum_{s=1}^{t} \psi_{ts} E_{s-1} = O(1).$$

Then e_n is bounded as $h \longrightarrow 0$, $n \longrightarrow \infty$, in the larger critical region $x_n = O(h^{-1/2})$, provided $r \geq 2$ with underlying assumptions (75), (76-i), (76-ii) and (77). Hence for a given A_2-stable usual method, the corresponding perturbed linear multistep method (32) applied to a model initial value problem of the form (71) with $Re\sqrt{\lambda} \leq 0$, the numerical solution $y_n = y(x_n) + e_n$, is bounded as $h \longrightarrow 0$, $n \longrightarrow \infty$, $x_n = O(h^{-1/2})$, under the assumptions (75),(76-i),(76-ii) and (77), provided $r \geq 2$. Hence the perturbed linear multistep method (32) is A_2-stable under these assumptions.

CHAPTER - 3

ERROR ANALYSIS OF THE OPTIMAL MULTISTEP METHOD FOR BOUNDARY VALUE PROBLEM

3.1 Introduction

In this chapter, we shall study certain theoretical aspects of the β-optimal multistep method, where optimization is done with respect to the β-coefficients, with prefixed α's, which can be used for the numerical solution of two point boundary value problems of the form:

(1) $$y'' + f(x,y) = 0, \qquad y(a) = A, \quad y(b) = B,$$

where $-\infty < a < b < \infty$, A and B are arbitrary constants, and the function $f(x,y)$ satisfies the following conditions :

(i) $f(x,y)$ is defined and continuous in the strip $a \le x \le b$, $-\infty < y < \infty$, where a and b are finite.

(ii) There exists a constant L such that for any $x \in [a,b]$ and any two numbers y and y^*

$$| f(x,y) - f(x,y^*) | \le L | y - y^* |.$$

In addition to satisfying the conditions (i) and (ii), $f(x,y)$ has continuous partial derivatives with respect to y. If

$$u_* = \inf_{a \le x \le b} \frac{\partial f}{\partial y} \qquad \text{and} \qquad u^* = \sup_{a \le x \le b} \frac{\partial f}{\partial y},$$

then we consider the following two categories of boundary value problems, with either $-\infty < u^* \le 0$, or $0 < u^* < \pi^2/(b-a)^2$.

Convergence analysis of a usual multistep method has been

given in Henrici [96], using monotone matrices, for solving a two point boundary value problem of M-type, for which $\frac{\partial f}{\partial y} \le 0$. Here we shall derive the convergence and the stability analysis of the β-optimal method, also using monotone matrices, for solving a two point boundary value problem of M-type, for which

$$-\infty < \frac{\partial f}{\partial y} < \pi^2/(b-a)^2.$$

For a multistep method of the form

$$(2) \qquad \sum_{i=0}^{k} \alpha_i \, y_{n-1+i} - h^2 \sum_{i=0}^{k} \beta_{i,n} \, f_{n-1+i} = 0; \qquad 1 \le n \le N-1,$$

where $f_m = f(x_m, y_m)$, adopted for the numerical solution of a two point boundary value problem of the form (1), as y_0 and y_N are being determined by the boundary conditions, the unknowns are y_1, y_2, ...,y_{N-1}. If the step number k of the difference equation is greater than two, new unknown values y_{-1} or y_N become introduced, for which there is no equation. This difficulty can be avoided by suitably modifying the difference equations near the boundary points. This situation does not arise, if k = 2, in (2) and if the associated difference operator has positive order p, then the difference equation (2) is an equation of the form

$$(3) \qquad \sum_{i=0}^{2} \alpha_i y_{n-1+i} - h^2 \sum_{i=0}^{2} \beta_i f_{n-1+i} = 0,$$

where $\alpha_0 = -1$, $\alpha_1 = 2$, $\alpha_2 = -1$ and $\beta_0 + \beta_1 + \beta_2 = 1$. Let p denote the order of the linear difference operator associated with the difference scheme (3).

If $\beta_0 = 0$, $\beta_1 = 1$, $\beta_2 = 0$ in (3), it becomes Stormer's method with function evaluation at one point, given by

(4) $$- y_{n-1} + 2y_n - y_{n+1} - h^2 f_n = 0,$$

with p = 2, as the order of the associated difference operator.

If $\beta_0 = \frac{1}{12}$, $\beta_1 = \frac{10}{12}$, $\beta_2 = \frac{1}{12}$ in (3), it becomes Cowell's method with function evaluation at three points, given by

(5) $$- y_{n-1} + 2y_n - y_{n+1} - h^2\{\frac{1}{12}f_{n-1} + \frac{10}{12}f_n + \frac{1}{12}f_{n+1}\} = 0,$$

p = 4, being the order of the associated difference operator. The β-optimal method corresponding to the schemes (4) and (5) will be the subject of study in this chapter.

In section 3.2, we shall state some known results which are required in the analysis of the following sections. In section 3.3, we shall derive the relation between the β- coefficients of the optimal method and those of the corresponding usual methods (4) and (5). In section 3.4, we shall describe the monotone properties of some matrices which are needed in the analysis of the succeeding sections. In section 3.5, we discuss the convergence analysis of the β-optimal methods corresponding to the usual methods (4) and (5). In section 3.6, we shall derive the order of convergence of a system of nonlinear difference equations with optimal β-coefficients for solving a nonlinear boundary value problem by Newton's method. In section 3.7, we shall discuss the stability analysis of the β-optimal methods and of the corresponding usual methods (4) and (5).

3.2 Some Known Results On Linear Multistep Method For BVP

In this section, we shall state some known results on linear multistep methods adopted for the numerical solution of a two point boundary value problem of the form (1).

The linear difference operator associated with the multistep method (2) for solving a boundary value problem (1) is given by

$$L\,[y(x);h] = \sum_{i=0}^{k} \alpha_i y(x+ih) + h^2 \sum_{i=0}^{k} \beta_i y''(x+ih).$$

Let $L\,[y(x);h]$ be applied to functions which have continuous derivatives of sufficiently high order. Then expanding by Taylor series, in powers of h, we obtain

$$L\,[y(x);h] = C_0 y(x) + C_1 y'(x)h + \dots\dots\dots + C_q y^{(q)}(x)h^q + \dots\dots$$

where the coefficients C_q $(q = 1,2,\dots.)$ are independent of $y(x)$.

$$C_0 = \sum_{i=0}^{k} \alpha_i, \qquad C_1 = \sum_{i=0}^{k} i\alpha_i$$

$$C_q = \frac{1}{q!}\sum_{i=0}^{k} i^q \alpha_i + \frac{1}{(q-2)!}\sum_{i=0}^{k} i^{q-2}\beta_i, \qquad q = 2,3,\dots\dots .$$

<u>Definition 1:</u> (Henrici [96]) The order p of the difference operator $L\,[y(x);h]$ is defined as the unique integer such that

$$C_q = 0,\ q = 0,1,\dots,\ p+1; \quad C_{p+2} \neq 0.$$

<u>Lemma 1:</u> (Henrici [96]) Let $L\,[y(x);h]$ be a difference operator of order $p > 0$. There exists a constant $G > 0$, depending only on L, such that

$$| L[y(x);h] | \le h^{p+2}GY, \quad a \le x, \quad x+kh \le b,$$

for all functions $y(x)$ having a continuous derivative of order $p+2$ in $[a,b]$, where $Y = \max_{a \le x \le b} |y^{(p+2)}(x)|$.

<u>Theorem 1:</u> (Theorem 7.2, Henrici [96]) Let $A = (a_{ij})$ be a matrix of order $n \ge 2$ and W be the set of the first n integers. Then A is irreducible if and only if for any two integers i and j, $i \in W$, $j \in W$, there exists a sequence of nonzero elements of A of the form

$$\{a_{i,i_1}, a_{i_1,i_2}, a_{i_2,i_3}, \ldots\ldots\ldots, a_{i_{m-1},j}\}.$$

<u>Corollary 1:</u> (Corollary of Theorem 7.2, Henrici [96]) A tridiagonal matrix $A = (a_{ij})$ is irreducible if and only if

$$a_{i,i-1} \ne 0, \; i = 2,3,\ldots,n; \text{ and } a_{i,i+1} \ne 0, \quad i = 1,2,\ldots,n-1.$$

Let z be a vector. By the notation $z \ge 0$, we mean that all the components z_i of the vector z, satisfy $z_i \ge 0$. Let us denote the null matrix by $\underline{0}$.

<u>Definition 2:</u> (Henrici [96]) A matrix A, with real elements is called monotone, if $Az \ge 0$implies $z \ge 0$.

<u>Theorem 2:</u> (Theorem 7.3, Henrici [96]) A matrix A is monotone if and only if the elements of the inverse matrix A^{-1} are non-negative.

<u>Theorem 3:</u> (Theorem 7.2, Henrici [96]) Let the matrix $A = (a_{ij})$ be irreducible and satisfy the conditions

(i) $$a_{ij} \le 0, \quad i \ne j; \quad i,j = 1,2,\ldots\ldots,n,$$

(ii) $$\sum_{j=1}^{n} a_{ij} \begin{cases} \ge 0, & i = 1,2,\ldots.,n, \\ > 0, & \text{for at least one } i. \end{cases}$$

Then A is a monotone matrix.

Theorem 4: (Theorem 7.5, Henrici [96]) Let the matrices A and B be monotone and assume that

$$A - B \ge \underline{0}$$

Then

$$B^{-1} - A^{-1} \ge \underline{0}.$$

Definition 3: (Definition 1.7, Varga [188]) An n x n complex matrix $A = (a_{ij})$ is diagonally dominant if

$$|\, a_{ii} \,| \ge \sum_{\substack{j=1 \\ j \ne i}}^{n} |\, a_{ij} \,| \quad \text{for all } 1 \le i \le n.$$

Corollary 2: (Corollary 1 of Theorem 3.11, Varga [188]) If $A = (a_{ij})$ is a real, irreducibly diagonally dominant $n \times n$ matrix with $a_{ij} \le 0$ for all $i \ne j$, and $a_{ii} > 0$ for all $1 \le i \le n$, then $A^{-1} > \underline{0}$, where $\underline{0}$ is the null matrix.

We define $\|v\|$, a norm of a vector $v = (v_1,v_2,\ldots,v_n)^T$, by

$$\|v\| = \max_{1 \le i \le n} |v_i|$$

and $\|A\|$, a norm of a matrix $A = (a_{ij})_{i,j=1(1)n}$, by

$$\|A\| = \max_{1 \le i \le n} \sum_{j=1}^{n} |a_{ij}|.$$

Lemma 2: (Lemma 7.1, Henrici [188]) Let A be a matrix such that $\|A\| = k < 1$, and let I denote the unit matrix. Then the matrix $(I - A)^{-1}$ exists, and

$$\|(I - A)^{-1}\| \le \frac{1}{1 - k}.$$

The following lemma gives an upper bound for the local truncation error of the β-optimal method. The proof follows along the lines of the proof of Lemma 4, in section 2.3.

Lemma 3: Let

$$L\,[y(x);h] = \sum_{i=0}^{k} \alpha_{k-i} y(x+(k-i)h) + h^2 \sum_{i=0}^{k} \beta_{k-i} y''(x+(k-i)h)$$

be the difference operator of a k-step usual method of order $p > 0$ and let

$$\hat{L}\,[y(x);h] = \sum_{i=0}^{k} \alpha_{k-i} y(x+(k-i)h) + h^2 \sum_{i=0}^{k} \hat{\beta}_{k-i,x} y''(x+(k-i)h)$$

be the difference operator of the corresponding β-optimal method, where $\hat{\beta}_{k-i,x}$; $0 \le i \le k$, are the optimal coefficients depending on x, corresponding to the usual coefficients β_{k-i}; $0 \le i \le k$. Let the exact solution y(x) of the differential equation have a continuous derivative of order p+2 for $x \in [a,b]$ and let

$$Y = \max_{\substack{a \le x \le b \\ 0 \le i \le p+2}} |\, y^{(i)}(x) \,|.$$

Then in Hilbert space, H, in which D_x^{p+2}, the representer of p+2-th derivative evaluation functional at x exists and is uniformly bounded on [a,b]

$$|\, \hat{L}\,[y(x);h] \,| \le h^{p+2} G^{*} Y, \qquad a \le x, \quad x+kh \le b,$$

where G^{*} is a positive constant.

3.3 Relation Between Optimal and Usual β-Coefficients

The following two lemmas relate the β-coefficients of the β-optimal multistep method and the corresponding usual multistep method.

Lemma 4: Let

(6) $$\sum_{i=-k}^{k} \alpha_i y_{n-i} - h^2 \sum_{j=-q}^{q} \beta_j f_{n-j} = 0, \quad k \le n \le N-k,$$

be a consistent usual method of order $p > 2q$, where α_i's and β_j's are symmetric in the sense that $\alpha_i = \alpha_{-i}$ and $\beta_j = \beta_{-j}$, for all i's and j's. If

$$\sum_{i=-k}^{k} \alpha_i y_{n-i} - h^2 \sum_{j=-q}^{q} \hat{\beta}_{j,n} f_{n-j} = 0, \quad k \le n \le N-k,$$

is the corresponding β-optimal method in a Hilbert space, H, in which D_x^{p+2}, the representer of p+2-th derivative evaluation functional at $x \in [a,b]$, exists and is uniformly bounded on [a,b], there holds

$$|\hat{\beta}_{j,n} - \beta_j| = O(h^2), \quad h \to 0, \quad j = -q(1)q,$$

uniformly for every n = k(1)N-k.

Proof: By the symmetry of the usual coefficients, the equations for C_q, given in Definition 1, show that actually $p \ge 2q+2$. Hence by Lemma 5 of Chapter 2, we have

$$|\hat{\beta}_{j,n} - \beta_j| = O(h^{p-(2q+1)+1}) = O(h^2), \quad h \to 0, \quad j = -q(1)q,$$

uniformly for every n =k(1)N-k.

Remark : It is easily seen that at least the highest degree polynomial precision usual method of type (6) has order p indeed $\geq$ 2q+2.

It follows from Lemma 4, that in case of Cowell's method (5),

$$|\hat{\beta}_{in} - \beta_i| = \phi_{in} h^2, \qquad i = 0,1,2; \quad 1 \leq n \leq N-1,$$

where ϕ_{in}, $i = 0,1,2$; $1 \leq n \leq N-1$ are some constants.

Let $\Phi = \max\limits_{1 \leq n \leq N-1} \left| \sum_{i=0}^{2} \phi_{in} \right|.$

Then $|(\hat{\beta}_{in} - \beta_i)| \leq \Phi h^2, \qquad i = 0,1,2; \quad 1 \leq n \leq N-1,$

where $\beta_0=1/12$, $\beta_1=10/12$, $\beta_2=1/12$. Thus we get the inequalities

$$\frac{1}{12} - \Phi h^2 \leq \hat{\beta}_{in} \leq \frac{1}{12} + \Phi h^2, \quad \text{for} \quad i = 0,2 \quad \text{and}$$

$$\frac{10}{12} - \Phi h^2 \leq \hat{\beta}_{1n} \leq \frac{10}{12} + \Phi h^2.$$

So, $\hat{\beta}_{in} \geq 0, \quad \text{for} \quad i = 0,1,2$

if, $\frac{1}{12} - \Phi h^2 \geq 0$ and $\frac{10}{12} - \Phi h^2 \geq 0$, i.e. if, $\Phi h^2 \leq \frac{1}{12}$.

Hence we have the following:

Corollary 3: Assume that $|\hat{\beta}_{in} - \beta_i| \leq \Phi h^2$, $1 \leq n \leq N-1$, where $\hat{\beta}_{in}$ are the optimal coefficients corresponding to the usual coefficients β_i, $i = 0(1)2$, of Cowell's method (5). Then in a Hilbert space, H, in which D_x^6, the representer of 6-th derivative evaluation functional at x, exists and is uniformly bounded on [a,b], $\hat{\beta}_{in} \geq 0$, $i = 0,1,2$; $1 \leq n \leq N-1$, if $\Phi h^2 \leq \frac{1}{12}$.

It also follows from Lemma 4, that in case of Stormer's method (4), with $\beta_1 = 1$,

$$|\hat{\beta}_{1n} - 1| = \theta_{n,h} h^2, \quad i = 0,1,2; \quad 1 \le n \le N-1,$$

where $\theta_{n,h}$, $1 \le n \le N-1$ are some constants.

Let $\quad \Theta = \max\limits_{1 \le n \le N-1} |\theta_{n,h}|.$

Then $\quad |(\hat{\beta}_{1n} - 1)| \le \Theta\, h^2, \qquad i = 0,1,2; \quad 1 \le n \le N-1.$

So, $\quad \hat{\beta}_{1n} \ge 0, \quad$ if $\Theta\, h^2 \le 1$.

Thus we have the following:

Corollary 4: Assume that $|\hat{\beta}_{1n} - 1| \le \Theta h^2$, $1 \le n \le N-1$, where $\hat{\beta}_{1n}$ are the optimal coefficients corresponding to the usual coefficients $\beta_1 = 1$, of Stormer's method (4). Then in a Hilbert space, H, in which D_x^4, the representer of 4-th derivative evaluation functional at $x \in [a,b]$, exists and is uniformly bounded on $[a,b]$, $\hat{\beta}_{1n} \ge 0$, $1 \le n \le N-1$, if $\Theta\, h^2 \le 1$.

In the following lemma, we are showing that in $H^2(C_r)$-space, and in $L^2(\hat{C}_r)$-space, the optimal β-coefficient indeed differ from the corresponding usual β-coefficient of Stormer's method by $O(h^2)$, what it is expected, by Lemma 4. However, in $H^{(3)}_{a,b}$ space, in which D_x^4, the representer for the 4-th derivative evaluation functional does not exist, this difference is of $O(h)$.

Lemma 5 : Let

$$(10) \qquad \sum_{i=0}^{2} \alpha_i y_{n-1+i} - h^2\, \hat{\beta}_{1,n} f_n = 0; \qquad 1 \le n \le N-1$$

be the β-optimal method, corresponding to Stormer's usual method (4), where $\hat{\beta}_{1,n}$; $1 \le n \le N-1$ are the optimal coefficients corresponding to the usual coefficient $\beta_1 = 1$, at the point x_n.

Then in $H^2(C_r)$ space and $L^2(\hat{C}_r)$ space,

$|\hat{\beta}_{1,n} - \beta_1| = O(h^2)$, $h \longrightarrow 0$, uniformly for every $n = 1,2,..,N-1$.

However, in $H^{(3)}_{a,b}$ space,

$|\hat{\beta}_{1,n} - \beta_1| = O(h)$, $h \longrightarrow 0$, uniformly for every $n = 1,2,..,N-1$.

Proof: From the normal equation (11) of Chapter 1, we can obtain $\hat{\beta}_{1,n}$, at a point x_n, $1 \le n \le N-1$, which is given by

(11) $$\hat{\beta}_{1,n} = -\frac{1}{h^2}\frac{\sum_{i=0}^{2} \alpha_i D2(x_{n-1+i}, \bar{x}_n)}{D2''(x_n, \bar{x}_n)},$$

where $D2(t,\bar{z}) = \frac{\partial^2}{\partial z^2} K(t,\bar{z})$; and $D2''(t,\bar{z}) = \frac{\partial^2}{\partial t^2} D(t,\bar{z})$.

Case 1: In $H^2(C_r)$ space :

$$K(t,\bar{z}) = \frac{1}{\pi}\frac{r}{(r^2 - t\bar{z})}, \qquad D2(t,\bar{z}) = \frac{1}{\pi}\frac{rt^2}{(r^2 - t\bar{z})^3},$$

and $$D2''(t,\bar{z}) = \frac{1}{\pi}\frac{2r\,[r^2(r^2 + 4t\bar{z}) + t^2\bar{z}^2]}{(r^2 - t\bar{z})^5}.$$

Putting the values of $K(t,\bar{z})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ in (11), we get $\hat{\beta}_{1,n}$ = Num /Din , where

$$\text{Num} = -\frac{1}{h^2}\left[-\frac{2rx^2_{n-1}}{(r^2 - x_{n-1}x_n)^3} + \frac{4rx^2_n}{(r^2 - x^2_n)^3} - \frac{2rx^2_{n+1}}{(r^2 - x_{n+1}x_n)^3}\right],$$

$$\text{Din} = \frac{4r\,[r^2(r^2 + 4x^2_n) + x^4_n]}{(r^2 - x^2_n)^5},$$

writing $x_n = x$, and $$C = \frac{(r^2 - x^2)^2}{2h^2(r^4 + 4r^2x^2 + x^4)},$$

$$\hat{\beta}_{1,n} = C\left[\frac{(x-h)^2(r^2-x^2)^3}{(r^2-x^2+xh)^3} + \frac{(x+h)^2(r^2-x^2)^3}{(r^2-x^2-xh)^3} - 2x^2\right]$$

$$= C\left[(x-h)^2\left\{1+\frac{hx}{r^2-x^2}\right\}^{-3} + (x+h)^2\left\{1-\frac{hx}{r^2-x^2}\right\}^{-3} - 2x^2\right]$$

$$= C\left[2h^2 + 4hx\frac{3hx}{r^2-x^2} + 2(x^2+h^2)\frac{6h^2x^2}{(r^2-x^2)^2} + 4hx\frac{10h^3x^3}{(r^2-x^2)^3}\right.$$

$$\left. + 2(x^2+h^2)\frac{15h^4x^4}{(r^2-x^2)^4} + 4hx\frac{21h^5x^5}{(r^2-x^2)^5} + \ldots\ldots\ldots\right]$$

$$= 2h^2 C\left[1 + \frac{6x^2}{r^2-x^2} + \frac{6x^2(x^2+h^2)}{(r^2-x^2)^2} + \frac{20h^2x^4}{(r^2-x^2)^3} + \frac{15h^2x^4(x^2+h^2)}{(r^2-x^2)^4}\right.$$

$$\left. + \frac{42h^4x^6}{(r^2-x^2)^5} + \ldots\ldots\ldots\right]$$

$$= \frac{(r^2-x^2)^2}{(r^4+4r^2x^2+x^4)}\left[\frac{(r^4+4r^2x^2+x^4)}{(r^2-x^2)^2} + \frac{h^2(6r^4x^2+8r^2x^4+x^6)}{(r^2-x^2)^4} + O(h^4)\right]$$

$$= 1 + h^2\frac{(6r^4x^2+8r^2x^4+x^6)}{(r^2-x^2)^2(r^4+4r^2x^2+x^4)} + O(h^4).$$

<u>Case 2</u> : In $L^2(\hat{C}_r)$ space :

$$K(t,\bar{z}) = \frac{1}{\pi}\frac{r^2}{(r^2-t\bar{z})^2}, \qquad D2(t,z) = \frac{1}{\pi}\frac{6r^2t^2}{(r^2-t\bar{z})^4},$$

and $$D2''(t,\bar{z}) = \frac{1}{\pi}\frac{12r^2\,[r^2(r^2+6t\bar{z}) + 3t^2z^2]}{(r^2-t\bar{z})^6}.$$

Putting the values of $K(t,\bar{z})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ in (11), we get $\hat{\beta}_{1,n}$ = Num /Din . Now

$$\text{Num} = -\frac{1}{h^2}\left[-\frac{6r^2x_{n-1}^2}{(r^2 - x_{n-1}x_n)^4} + \frac{12r^2x_n^2}{(r^2 - x_n^2)^4} - \frac{6r^2x_{n+1}^2}{(r^2 - x_nx_{n+1})^4}\right],$$

$$\text{Din} = \frac{12r^2[r^2(r^2 + 6x_n^2) + 3x_n^4]}{(r^2 - x_n^2)^6},$$ So that

writing $x_n = x$, and $C = \dfrac{(r^2 - x^2)^2}{2h^2(r^4 + 6r^2x^2 + 3x^4)}$,

$$\hat{\beta}_{1,n} = C\left[\frac{(x-h)^2(r^2 - x^2)^4}{(r^2 - x^2 + hx)^4} + \frac{(x+h)^2(r^2 - x^2)^4}{(r^2 - x^2 - hx)^4} - 2x^2\right]$$

$$= C\left[(x-h)^2\left\{1 + \frac{hx}{r^2 - x^2}\right\}^{-4} + (x+h)^2\left\{1 - \frac{hx}{r^2 - x^2}\right\}^{-4} - 2x\right]$$

$$= C\Bigg[2h^2 + 4hx\frac{4hx}{r^2-x^2} + 2(x^2+h^2)\frac{10h^2x^2}{(r^2-x^2)^2} + 4hx\frac{20h^3x^3}{(r^2-x^2)^3}$$

$$+ 2(x^2+h^2)\frac{35h^4x^4}{(r^2-x^2)^4} + 4hx\frac{56h^5x^5}{(r^2-x^2)^5} + \ldots\ldots\ldots\ldots\Bigg]$$

$$= 2h^2C\left[1 + \frac{8x^2}{r^2-x^2} + \frac{10x^2(x^2+h^2)}{(r^2-x^2)^2} + \frac{40h^2x^4}{(r^2-x^2)^3} + \frac{35h^2x^4(x^2+h^2)}{(r^2-x^2)^4} + \ldots\right]$$

$$= \frac{(r^2-x^2)^2}{(r^4+6r^2x^2+3x^4)}\left[\frac{(r^4+6r^2x^2+3x^4)}{(r^2 - x^2)^2} + \frac{5h^2(2r^4x^2+4r^2x^4+x^6)}{(r^2-x^2)^4} + O(h^4)\right]$$

$$= 1 + h^2\frac{5(2r^4x^2+4r^2x^4+x^6)}{(r^2-x^2)^2(r^4+6r^2x^2+3x^4)} + O(h^4).$$

<u>Case 3</u> : In $H^{(3)}_{a,b}$ space :

$$K(t,s)=\begin{cases} \dfrac{1}{\alpha_0}+\dfrac{1}{5!}\left(\dfrac{t-a}{b-a}\right)^5+\displaystyle\sum_{i=1}^{2}\dfrac{1}{i!^2\alpha_i}\left(\dfrac{s-a}{b-a}\right)^i\left[\left(\dfrac{t-a}{b-a}\right)^i+\dfrac{(-1)^{2-i}\alpha_i\, i!}{(5-i)!}\left(\dfrac{t-a}{b-a}\right)^{5-i}\right] \\ \qquad\qquad\qquad\qquad \text{for } a \le t \le s, \\ \dfrac{1}{\alpha_0}+\dfrac{1}{5!}\left(\dfrac{s-a}{b-a}\right)^5+\displaystyle\sum_{i=1}^{2}\dfrac{1}{i!^2\alpha_i}\left(\dfrac{t-a}{b-a}\right)^i\left[\left(\dfrac{s-a}{b-a}\right)^i+\dfrac{(-1)^{2-i}\alpha_i\, i!}{(5-i)!}\left(\dfrac{s-a}{b-a}\right)^{5-i}\right] \\ \qquad\qquad\qquad\qquad \text{for } a \le t \le s. \end{cases}$$

$$D2(t,s)=\begin{cases} \dfrac{1}{(b-a)^2}\left[\dfrac{1}{3!}\left(\dfrac{t-a}{b-a}\right)^3+\dfrac{1}{2!\alpha_2}\left(\dfrac{t-a}{b-a}\right)^2\right], & \text{for } a \le t \le s, \\ \dfrac{1}{(b-a)^2}\left[\dfrac{1}{3!}\left(\dfrac{s-a}{b-a}\right)^3-\dfrac{1}{2!}\left(\dfrac{s-a}{b-a}\right)^2\left(\dfrac{t-a}{b-a}\right)+\dfrac{1}{2!}\left(\dfrac{t-a}{b-a}\right)^2\left(\dfrac{s-a}{b-a}\right)+\dfrac{1}{2!\alpha_2}\left(\dfrac{t-a}{b-a}\right)^2\right], & \text{for } s \le t \le b \end{cases}$$

$$D2''(t,s)=\begin{cases} \dfrac{1}{(b-a)^4}\left[\left(\dfrac{t-a}{b-a}\right)+\dfrac{1}{\alpha_2}\right], & \text{for } a \le t \le s, \\ \dfrac{1}{(b-a)^4}\left[\left(\dfrac{s-a}{b-a}\right)+\dfrac{1}{\alpha_2}\right], & \text{for } s \le t \le b, \end{cases}$$

Putting the values of $K(t,\bar{z})$, $D2(t,\bar{z})$, and $D2''(t,\bar{z})$ in (11), and writing $x_n = x$, we get

$$\begin{aligned} \text{Num} = -\frac{1}{h^2}\frac{1}{(b-a)^2}\Bigg[& -\left\{\frac{1}{3!}\left(\frac{x-h-a}{b-a}\right)^3+\frac{1}{2!\alpha_2}\left(\frac{x-h-a}{b-a}\right)^2\right\} \\ & + 2\left\{\frac{1}{3!}\left(\frac{x-a}{b-a}\right)^3+\frac{1}{2!\alpha_2}\left(\frac{x-a}{b-a}\right)^2\right\} \\ & - \left\{\frac{1}{3!}\left(\frac{x-a}{b-a}\right)^3-\frac{1}{2!}\left(\frac{x-a}{b-a}\right)^2\left(\frac{x+h-a}{b-a}\right)+\frac{1}{2!}\left(\frac{x+h-a}{b-a}\right)^2\left(\frac{x-a}{b-a}\right)+\frac{1}{2!\alpha_2}\left(\frac{x+h-a}{b-a}\right)^2\right\}\Bigg] \end{aligned}$$

$$= \frac{1}{h^2}\frac{(x-a)^2}{(b-a)^5}\Bigg[\left\{\frac{(x-a)}{3!}\left(1-\frac{h}{x-a}\right)^3+\frac{(b-a)}{2!\alpha_2}\left(1-\frac{h}{x-a}\right)^2\right\}$$

$$-2\left\{\frac{(x-a)}{3!}+\frac{b-a}{2!\alpha_2}\right\}$$

$$+\left\{\frac{(x-a)}{3!}-\frac{(x-a)}{2!}\left(1+\frac{h}{x-a}\right)+\frac{(x-a)}{2!}\left(1+\frac{h}{x-a}\right)^2+\frac{(b-a)}{2!\alpha_2}\left(1+\frac{h}{x-a}\right)^2\right\}\Bigg]$$

$$= \frac{1}{h^2}\frac{(x-a)^2}{(b-a)^5}\left[h^2\left\{\frac{2}{2!(x-a)}+\frac{2(b-a)}{2!\alpha_2(x-a)^2}\right\}-\frac{h^3}{3!(x-a)^2}\right]$$

$$= \frac{1}{h^2}\frac{(x-a)^2}{(b-a)^5}\left[\frac{h^2}{(x-a)^2}\left((x-a)+\frac{1}{\alpha_2}(b-a)\right)-\frac{h^3}{3!(x-a)^2}\right].$$

$$\text{Din} = \frac{1}{(b-a)^4}\left(\frac{x-a}{b-a}+\frac{1}{\alpha_2}\right) = \frac{1}{(b-a)^5}\left(x-a+\frac{1}{\alpha_2}(b-a)\right).$$

Hence, $$\hat{\beta}_{1,n} = 1-\frac{h}{3!\left(x-a+\frac{1}{\alpha_2}(b-a)\right)}.$$

3.4 Some Auxiliary Results

In this section, we establish some results required in the following sections. The notations for some specific matrices valid throughout this chapter are as follows:

Definition 4: $J = (j_{n,m})_{n,m=1}^{N-1}$ is a tridiagonal matrix with

$j_{n,n-1} = -1,$ for $2 \le n \le N-1;$

$j_{n,n} = 2,$ for $1 \le n \le N-1;$

$j_{n,n+1} = -1,$ for $1 \le n \le N-2.$

Definition 5: $\hat{D} = \text{diag}\,(\hat{\beta}_{1,1},\hat{\beta}_{1,2},\ldots\ldots\ldots,\hat{\beta}_{1,N-1}),$

where $\hat{\beta}_{1,n}$, $1\le n\le N-1$ are the optimal β-coefficients at the point x_n corresponding to the usual β-coefficient $\beta_1 = 1$ in Stormer's method.

<u>Definition 6</u>: $\hat{P} = (\hat{p}_{i,j})_{i,j=1}^{N-1}$ is a tridiagonal matrix with

$$\hat{p}_{i,i-1} = \hat{\beta}_{0,i}, \qquad \text{for } 2 \le i \le N-1;$$

$$\hat{p}_{i,i} = \hat{\beta}_{1,i}, \qquad \text{for } 1 \le i \le N-1;$$

$$\hat{p}_{i,i+1} = \hat{\beta}_{2,i}, \qquad \text{for } 1 \le i \le N-1.$$

where $\hat{\beta}_{i,n}$, $i = 0,1,2$; $1\le n \le N-1$ are the optimal β-coefficients at the point x_n corresponding to the usual β-coefficients $\beta_0 = \frac{1}{12}$, $\beta_1 = \frac{10}{12}$, $\beta_2 = \frac{1}{12}$, in Cowell's method.

<u>Definition 7</u>: $U = \text{diag}\,\{u_1, u_2, \ldots\ldots\ldots, u_{N-1}\}$,

where $u_i = \frac{\partial}{\partial y} f\,(x_i,\ w_i + \xi_i[v_i - w_i])$, $0 < \xi_i < 1$; $1 \le i \le N-1$, v_i and w_i are any two net functions.

<u>Definition 8</u>: $U_* = u_* I$, where $u_* = \inf\limits_{a\le x\le b} \frac{\partial f}{\partial y}$.

<u>Definition 9</u>: $U^* = u^* I$, where $u^* = \sup\limits_{a\le x\le b} \frac{\partial f}{\partial y}$.

<u>Definition 10:</u> $P = (p_{ij})_{i,j=1}^{N-1}$ is a tridiagonal matrix with

$$p_{ii} = \frac{10}{12}, \qquad \text{for } 1 \le i \le N-1;$$

$$p_{i,i-1} = \frac{1}{12}; \qquad \text{for } 2 \le i \le N-1;$$

$$p_{i,i+1} = \frac{1}{12}; \qquad \text{for } 1 \le i \le N-2.$$

<u>Definition 11</u> : $T = (t_{ij})_{i,j=1}^{N-1}$ is a tridiagonal matrix with all the components of its tridiagonal part as 1.

I is the identity matrix and $\underline{0}$ is the null matrix.

In the case of Cowell's method (5), according to Corollary 3, let $\hat{\beta}_{in} - \beta_i = \phi_{in} h^2$, for $i = 0,1,2;\ 1 \le n \le N-1$.

<u>Definition 12:</u> $\hat{\phi} = (\hat{\phi}_{ij})_{i,j=1}^{N-1}$ is a tridiagonal matrix, where

$$\hat{\phi}_{ii-1} = \phi_{01}, \quad 2 \le i \le N-1;$$
$$\hat{\phi}_{ii} = \phi_{11}, \quad 1 \le i \le N-1;$$
$$\hat{\phi}_{ii+1} = \phi_{21}, \quad 1 \le i \le N-2.$$

and $\|\hat{\phi}\| = \Phi$.

In the case of Stormer's method (4), according to Corollary 4, let $\hat{\beta}_{1n} - 1 = \theta_n h^2$, for $1 \le n \le N-1$.

<u>Definition 13:</u> $\hat{\theta} = \mathrm{diag}\{\theta_1, \theta_2, \ldots\ldots, \theta_{N-1}\}$, and $\|\hat{\theta}\| = \Theta$.

Let us recall Corollary 3 and Corollary 4 and establish the following lemmas.

<u>Lemma 6</u> : If $-\infty < u^* \le 0$, then $J - h^2\hat{D}U$ is monotone matrix for all h, provided $\Theta h^2 \le 1$.

<u>Proof</u> : $J - h^2\hat{D}U = (s_{nm})_{n,m=1}^{N-1}$ is irreducible, since for $n \ne m$ such that $|n-m|=1$, $s_{nm} = -1\ (\ne 0)$, and we have

$$\sum_{m=1}^{N-1} s_{nm} = \begin{cases} 1-h^2\hat{\beta}_{1,1}\,u_1 \ge 1 - h^2\,\hat{\beta}_{1,1}\,u^* > 0; & \text{for } n = 1 \\ 1-h^2\hat{\beta}_{1,N-1}\,u_{N-1} \ge 1 - h^2\,\hat{\beta}_{1,N-1}\,u^* > 0; & \text{for } n = N-1 \\ -h^2\,\hat{\beta}_{1,n}\,u_n \ge -h^2\,\hat{\beta}_{1,n}\,u^* \ge 0; & \text{for } 2 \le n \le N-2 \end{cases}$$

provided, $\hat{\beta}_{1,n} \ge 0$, for $1 \le n \le N-1$, which would be the case if $\Theta h^2 \le 1$, by Corollary 4. Hence, by Theorem 3, the lemma follows.

<u>Lemma 7</u> : If $0 < u^* < \pi^2/(b-a)^2$, then $J - h^2\hat{D}U$ is monotone matrix for all $h < H_0$; where H_0 is the smallest positive root of the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2 \frac{\pi H}{2(b-a)} = 0,$$

provided $\Theta h^2 \le 1$.

<u>Proof</u>: $J - h^2\hat{D}U$ is irreducible, since its off-diagonal elements of the tridiagonal part are -1, that is nonzero. Following Chawla [45], we can write

$$U = U^- + U^+; \quad \text{where} \quad U^- \le \underline{0} \quad \text{and} \quad U^+ > \underline{0}.$$

Then

$$J - h^2\hat{D}U = J - h^2\hat{D}(U^- + U^+) = (J - h^2\hat{D}U^-) - h^2\hat{D}U^+$$

$$= \hat{M} - h^2\hat{D}U^+ = \hat{M}\,(I - h^2\hat{M}^{-1}\hat{D}U^+), \quad \text{where } \hat{M} = J - h^2\hat{D}U^-.$$

By Lemma 6, $\hat{M}$ is monotone matrix provided $\Theta h^2 \le 1$. $J - h^2\hat{D}U$ will be monotone matrix, if $I - h^2\hat{M}^{-1}\hat{D}U^+$ is so. $I - h^2\hat{M}^{-1}\hat{D}U^+$ will be monotone matrix if its spectral radius, $\rho(h^2\hat{M}^{-1}\hat{D}U^+) < 1$.

Now, $\hat{M} \ge J$, if $\hat{D} \ge \underline{0}$, which would be the case if $\Theta h^2 \le 1$, according to Corollary 4. J is also a monotone matrix. Hence, by Theorem 4, we have

$$\hat{M}^{-1} \le J^{-1}, \quad \text{if } \Theta h^2 \le 1.$$

Let us use the spectral radius. Then

$$\rho(h^2\hat{M}^{-1}\hat{D}U^+) \le h^2u^*\,\rho(J^{-1}) \max_{1 \le n \le N-1} |\hat{\beta}_{1,n}|$$

since, $\rho(J^{-1}) = \dfrac{1}{4\sin^2 \dfrac{\pi h}{2(b-a)}}$, we get

$$\rho(h^2\hat{M}^{-1}\hat{D}U^+) \le \frac{h^2u^*}{4\sin^2 \dfrac{\pi h}{2(b-a)}}(1 + \Theta h^2) = g(h), \text{ say.}$$

$$\lim_{H\to 0} g(H) = \frac{u^*(b-a)^2}{\pi^2} < 1, \quad \text{and} \quad \lim_{H\to 2(b-a)} g(H) = \infty.$$

Hence g assumes the value 1, at some h in (0, 2(b-a)). Let H_0 denote the smallest positive root of the equation g(H) = 1, i.e.,

$$H^2u^*(1 + \Theta H^2) - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

Hence for all $h < H_0$, $\rho(h^2\, \hat{M}^{-1}\hat{D}U^+) < 1$, and the matrix $I - h^2\hat{M}^{-1}\hat{D}U^+$ is monotone. Hence the lemma.

<u>Lemma 8</u> : If $-\infty < u^* \le 0$, then $J - h^2\hat{P}U$ is irreducible and monotone matrix for all $h < \sqrt{\frac{6}{-u_*}}$, provided $\Phi h^2 \le \frac{1}{12}$.

<u>Proof</u>. $J - h^2\hat{P}U = (t_{nm})_{n,m=1}^{N-1}$ will be an irreducible matrix, if the off diagonal elements of its tridiagonal part are nonzero, i.e. if, for $n \ne m$, such that $|n-m| = 1$, $t_{nm} = -1 - h^2\hat{\beta}_{i,n}u_m \ne 0$, for i = 0,2; $1 \le m,n \le N-1$. Since, $u_* \le u_m \le u^*$, for $1 \le m \le N-1$, and $\frac{1}{12} - \Phi h^2 \le \hat{\beta}_{i,n} \le \frac{1}{12} + \Phi h^2$; and $\hat{\beta}_{i,n} \ge 0$, i = 0,1,2; $1 \le n \le N-1$, provided $\Phi h^2 \le \frac{1}{12}$, by Corollary 3. Thus we get

$$-h^2\, \hat{\beta}_{i,n}u_m \le -h^2\, \hat{\beta}_{i,n}u_* \le -h^2(\frac{1}{12} + \Phi h^2)u_* \le \frac{-h^2u_*}{6};$$

for i = 0,1,2; $1 \le n \le N-1$.

Hence, the condition of irreducibility is satisfied

if, $\frac{-h^2u_*}{6} < 1$ i.e., if $h < \sqrt{\frac{6}{-u_*}}$.

Now, for $n \ne m$, such that $|n-m| = 1$, $t_{n,m} = -1 - h^2\hat{\beta}_{i,n}u_m \le 0$, for i = 0,2; $1 \le m,n \le N-1$, which is true by the condition of irreducibility. Now

$$\sum_{m=1}^{N-1} t_{n,m} = \begin{cases} -h^2(\hat{\beta}_{0,n}\, u_{n-1} + \hat{\beta}_{1,n}\, u_n + \hat{\beta}_{2,n}\, u_{n+1}) \\ \qquad \ge -h^2(\hat{\beta}_{0,n} + \hat{\beta}_{1,n} + \hat{\beta}_{2,n})\, u^* \ge 0, \quad \text{for } 2 \le n \le N-1, \\ 1 - h^2(\hat{\beta}_{1,1}u_1 + \hat{\beta}_{2,1}u_2) \ge 1 - h^2(\hat{\beta}_{1,1} + \hat{\beta}_{2,1})u^* > 0, \\ \qquad\qquad \text{for } n = 1, \\ 1 - h^2(\hat{\beta}_{0,N-1}\, u_{N-2} + \hat{\beta}_{1,N-1}\, u_{N-1}) \\ \qquad \ge 1 - h^2(\hat{\beta}_{0,N-1} + \hat{\beta}_{1,N-1})u^* > 0, \quad \text{for } n = N-1. \end{cases}$$

provided $\hat{\beta}_{i,n} \ge 0$, for $i = 0,1,2;\ 1 \le n \le N-1$, which holds provided $\Phi\, h^2 \le \frac{1}{12}$, by Corollary 3. Hence by Theorem 3, the lemma follows.

Lemma 9 Suppose, $0 < u^* < \pi^2/(b-a)^2$. If $u_* < 0$, then $J - h^2\hat{P}U$ is monotone for all $h < \min\{h_1, h_2\}$, and if $u_* > 0$, then $J - h^2\hat{P}U$ is monotone for all $h < h_2$, provided $\Phi h^2 \le \frac{1}{12}$, where $h_1 = \sqrt{\frac{6}{-u_*}}$, and h_2 is the smallest positive root of the equation :

$$H^2u^*[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2)4\sin^2 \frac{\pi H}{2(b-a)}] - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

Proof: $J - h^2\hat{P}U = (t_{nm})_{n,m=1}^{N-1}$ will be an irreducible matrix, if the off-diagonal elements of its tridiagonal part are nonzero, which is the case, if $-1 - h^2\hat{\beta}_{i,n}u_m \ne 0$, for $i = 0,2;\ 1 \le m,n \le N-1$.

By Corollary 3, $\frac{1}{12} - \Phi\, h^2 \le \hat{\beta}_{i,n} \le \frac{1}{12} + \Phi\, h^2$, and $\hat{\beta}_{i,n} \ge 0$, if $\Phi\, h^2 \le \frac{1}{12}$, for $i = 0,1,2;\ 1 \le n \le N-1$.

Now, $u_* \le u_m \le u^*$; for $1 \le m \le N-1$.

If $u_* \ge 0$, then $u_m \ge 0$.

So, $-h^2\, \hat{\beta}_{i,n}\, u_m \le 0$, if $\hat{\beta}_{i,n} \ge 0$, for $i = 0,2;\ 1 \le m,n \le N-1$.

Hence, $J - h^2 \hat{P} U$ is irreducible matrix provided $\Phi h^2 \le \frac{1}{12}$.

<u>If $u_* < 0$, then</u>

$$- h^2 \hat{\beta}_{i,n} u_m \le - h^2 \hat{\beta}_{i,n} u_* \le - h^2 u_* (\tfrac{1}{12} + \Phi h^2) \le \frac{-h^2 u_*}{6}$$

for $i = 0,2; \quad 1 \le n \le N-1,$ provided $\Phi h^2 \le \frac{1}{12}$. Hence, the matrix $J - h^2\hat{P}U$ is irreducible,

$$\text{if} \quad \frac{-h^2 u_*}{6} < 1, \quad \text{i.e., if} \quad h < \sqrt{\frac{6}{-u_*}} = h_1, \text{ say.}$$

Now for both the cases when $u_* \ge 0$, or $u_* < 0$, we proceed as follows.

As in Lemma 7, let $U = U^- + U^+$, where $U^- \le \underline{0}$ and $U^+ > 0$. Then $J - h^2\hat{P}U = \hat{M} - h^2\hat{P}U^+ = \hat{M}(I - h^2\hat{M}^{-1}\hat{P}U^+)$, where $\hat{M} = J - h^2\hat{P}U^-$.

By Lemma 8, $\hat{M}$ is irreducible and monotone for all $h < \sqrt{\frac{6}{-u_*}}$. $J-h^2\hat{P}U$ will be a monotone matrix if $I - h^2\hat{M}^{-1}\hat{P}U^+$ is so. $I - h^2\hat{M}^{-1}\hat{P}U^+$ will be a monotone matrix, if the spectral radius, $\rho(h^2\hat{M}^{-1}\hat{P}U^+) < 1$.

Now, $\hat{M} \ge J$, if $\hat{P} \ge 0$, which would be the case, if $\Phi h^2 \le \frac{1}{12}$, according to Corollary 3. Hence, by Theorem 4, we have

$$\hat{M}^{-1} \le J^{-1}, \qquad \text{if} \quad \Phi h^2 \le \frac{1}{12} .$$

Now by the definition of $\hat{P}$, P and T from Definitions 6, 10, 11 and using the fact that $|\beta_{in} - \beta_i| \le \Phi h^2 \quad i = 0,1,2; \quad 1 \le n \le N-1,$ we have

$$\hat{P} \le P + h^2\Phi T = (I - \frac{1}{12} J) + \Phi h^2(- J + 3I)$$

$$= (1 + 3\Phi h^2)I + (- \frac{1}{12} - \Phi h^2)J.$$

Since, J is a monotone matrix, $J^{-1} \ge \underline{0}$, by Theorem 2.

So, $\quad J^{-1} \hat{P} \le (1 + 3\Phi h^2)J^{-1} + (- \frac{1}{12} - \Phi h^2)I$

Using the spectral radius,

$$\rho(h^2\hat{M}^{-1}\hat{P}U^+) \le \rho(h^2J^{-1}\hat{P}U^+) \le h^2u^*\rho(J^{-1}\hat{P}),$$

Using the fact, $\rho(J^{-1}) = \dfrac{1}{4\sin^2\frac{\pi h}{2(b-a)}}$, we get

$$\rho(h^2\hat{M}^{-1}\hat{P}U^+) \le h^2u^*\left[(1+3\Phi h^2)\frac{1}{4\sin^2\frac{\pi h}{2(b-a)}}+(-\frac{1}{12}-\Phi h^2)\right] = g_1(h), \text{ say.}$$

$$\lim_{H\to 0} g_1(H) = \frac{u^*(b-a)^2}{\pi^2} < 1, \text{ and } \lim_{H\to 2(b-a)} g_1(H) = \infty.$$

Hence g_1 assumes the value 1, at some H in $(0,\ 2(b-a))$. Let h_2 denote the smallest positive root of the equation $g_1(H) = 1$, i.e., of the equation:

$$H^2u^*\left[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2)4\sin^2\frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

Hence for all $h < h_2$, $\rho(h^2\hat{M}^{-1}\hat{P}U^+) < 1$, and the matrix $I - h^2\hat{M}^{-1}\hat{P}U^+$ is monotone. Hence the lemma follows.

<u>Lemma 10</u> : If $-\infty < u^* \le 0$, then $J - h^2\hat{D}U^*$ is monotone matrix for all h, provided $\Theta h^2 \le 1$.

<u>Proof</u>: Proceeding as in Lemma 6, the result follows.

<u>Lemma 11</u> : If $0 < u^* < \pi^2/(b-a)^2$, then $J - h^2\hat{D}U^*$ is monotone matrix for all $h < H_0$, where H_0 is the smallest root of the equation :

$$H^2u^*(1 + \Theta H^2) - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

provided $\Theta h^2 \le 1$.

<u>Proof</u> : $J - h^2\hat{D}U^*$ is irreducible, since the off diagonal elements of its tridiagonal part are - 1, that is nonzero.

Since, $U^* > \underline{0}$, we can write,

$$J - h^2\hat{D}U^* = J(I - h^2J^{-1}\hat{D}U^*).$$

J being a monotone matrix, $J - h^2\hat{D}U^*$ will be a monotone matrix if $(I - h^2J^{-1}\hat{D}U^*)$ is so. Proceeding as in Lemma 7, $(I - h^2J^{-1}\hat{D}U^*)$ is a monotone matrix for all $h < H_0$. Hence the Lemma.

<u>Lemma 12</u> : If $-\infty < u^* \le 0$, then $J - h^2\hat{P}U^*$ is a monotone matrix for all $h < \sqrt{\dfrac{6}{-u^*}}$, provided $\Phi h^2 \le \frac{1}{12}$.

<u>Proof</u>: $J - h^2\hat{P}U^* = (t^*_{nm})^{N-1}_{n,m=1}$ will be an irreducible matrix, if the off-diagonal elements of its tridiagonal part are nonzero, which would be the case, if for $n \ne m$, such that $|n-m| = 1$,

$$t^*_{nm} = -1 - h^2\hat{\beta}_{i,n}u^* \ne 0, \quad i = 0,2; \quad 1 \le n \le N-1.$$

Now, since $u^* \le 0$, and by Corollary 3, $\hat{\beta}_{i,n} \ge 0$, if $\Phi h^2 \le \frac{1}{12}$,

$$-h^2\hat{\beta}_{i,n}u^* \le -h^2u^*\left(\frac{1}{12} + \Phi h^2\right) \le \frac{-h^2u^*}{6}.$$

So, the condition of irreducibility is satisfied

if, $\quad -\dfrac{h^2u^*}{6} < 1, \quad$ i.e., if $\quad h < \sqrt{\dfrac{6}{-u^*}}$.

For $n \ne m$, such that $|n-m| = 1$, $t^*_{nm} = -1 - h^2\hat{\beta}_{i,n}u^* \le 0$; for $i = 0,2$, by the condition of irreducibility. Now,

$$\sum_{m=1}^{N-1} t^*_{n,m} = \begin{cases} -h^2(\hat{\beta}_{0,n} + \hat{\beta}_{1,n} + \hat{\beta}_{2,n})u^* \ge 0, & \text{for } 2 \le n \le N-2; \\ 1 - h^2(\hat{\beta}_{1,1} + \hat{\beta}_{2,1})u^* > 0, & \text{for } n = 1; \\ 1 - h^2(\hat{\beta}_{0,N-1} + \hat{\beta}_{1,N-1})u^* > 0, & \text{for } n = N-1; \end{cases}$$

as $\hat{\beta}_{i,n} \ge 0$, provided $\Phi h^2 \le \frac{1}{12}$. Hence, by Theorem 4, the lemma follows.

<u>Lemma 13</u> : Suppose, $0 < u^* < \pi^2/(b-a)^2$, then $J - h^2PU^*$ is a monotone matrix for all $h < h_2$, where h_2 is the smallest positive root of the equation:

$$H^2u^*\left[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2)4\sin^2 \frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

provided $\Phi h^2 \le \frac{1}{12}$.

<u>Proof</u> : $J - h^2\hat{P}U^* = (t^*_{nm})^{N-1}_{n,m=1}$ is irreducible matrix, since the off-diagonal elements of its tridiagonal part are nonzero. By Corollary 3, we have:

$$\frac{1}{12} - \Phi h^2 \le \hat{\beta}_{i,n} \le \frac{1}{12} + \Phi h^2 \quad \text{and} \quad \hat{\beta}_{i,n} \ge 0, \quad \text{if } \Phi h^2 \le \frac{1}{12}.$$

So, $$- h^2\hat{\beta}_{i,n}u^* \le h^2u^*(\Phi h^2 - \frac{1}{12}) \le 0.$$

So, for $n \ne m$, such that $|n - m| \le 1$, $t^*_{nm} = - 1 - h^2\hat{\beta}_{i,n}u^* \ne 0$; for $i = 0,2$; $1 \le n \le N-1$. Now, since $U^* \ge 0$, we can write,

$$J - h^2\hat{P}U^* = J(I - h^2J^{-1}\hat{P}U^*).$$

J being a monotone matrix, $J - h^2\hat{P}U^*$ will be a monotone matrix if $(I - h^2J^{-1}\hat{P}U^*)$ is monotone. Proceeding as in Lemma 9, $(I- h^2J^{-1}\hat{P}U^*)$ is monotone for all $h < h_2$, provided $\Phi h^2 \le \frac{1}{12}$. Hence the Lemma.

<u>Lemma 14</u> : If $0 < u^* < \pi^2/(b-a)^2$, then $J - h^2U$ and $J - h^2U^*$ are monotone matrices for all $h < H_o$, where H_o is the smallest positive root of the equation

$$H^2u^* - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

In particular, the result holds for all $h < H_1$, where

$$H_1 = \sqrt{\frac{24(b-a)^2}{\pi^2}\left(1 - \sqrt{\frac{u^*(b-a)^2}{\pi^2}}\right)}.$$

Proof : $J - h^2U^* = J(I - J^{-1}h^2U^*)$, where $U^* > \underline{0}$. J is monotone matrix. So it is sufficient to prove that $(I-J^{-1}h^2U^*)$ is monotone matrix. The first assertion follows along the lines of the proof of Lemma 7. For the second assertion, we use the inequality $\sin^2 x \geq x^2(1 - x^2/6)^2$, $x \geq 0$, which is a slightly sharper form of the inequality used in Chawla [45].

Lemma 15: If $-\infty < u^* \leq 0$, then $J - h^2PU$ is monotone matrix for all $h < \sqrt{\frac{12}{-u_*}}$.

Proof : If $J - h^2PU = (\tilde{j}_{nm})_{n,m=1}^{N-1}$, then

$$\sum_{m=1}^{N-1} \tilde{j}_{n,m} = \begin{cases} -h^2(\frac{1}{12}u_{j-1} + \frac{10}{12}u_j + \frac{1}{12}u_{j+1}) \geq 0, & \text{for } 2 \leq n \leq N-1, \\ 1 - h^2(\frac{10}{12}u_2 + \frac{1}{12}u_3) > 0, & \text{for } n = 1, \\ 1 - h^2(\frac{1}{12}u_{N-2} + \frac{10}{12}u_{N-1}) > 0, & \text{for } n = N-1. \end{cases}$$

So, $J - h^2PU$ will be monotone, if for $n \neq m$, such that $|n - m| = 1$, $\tilde{j}_{n,m} \leq 0$, i.e., if $-1 - \frac{1}{12}h^2u_{i,i\pm 1} \leq -1 - \frac{1}{12}h^2u_* \leq 0$; i.e., if $h \leq \sqrt{\frac{12}{-u_*}}$. Hence the lemma.

Lemma 16: If $-\infty < u^* < 0$, then $J - h^2PU^*$ is monotone matrix for all $h < \sqrt{\frac{12}{-u^*}}$.

Proof : If $J - h^2PU^* = (\hat{j}_{nm})_{n,m=1}^{N-1}$, then

$$\sum_{m=1}^{N-1} \hat{j}_{n,m} = \begin{cases} -h^2u^* \geq 0, & \text{for } 2 \leq n \leq N-1; \\ 1 - h^2(\frac{10}{12} + \frac{1}{12})u^* > 0, & \text{for } n = 1, N-1. \end{cases}$$

So, $J - h^2PU^*$ will be monotone if for $n \neq m$, $\hat{j}_{n,m} \leq 0$, i.e., if $-1 - \frac{1}{12}h^2u^* \leq 0$; i.e., if $h \leq \sqrt{\frac{12}{-u^*}}$. Hence the lemma.

Lemma 17 : If $0 < u^* < \pi^2/(b-a)^2$, then $J - h^2PU^*$ is monotone matrix for all $h < h_0$, where h_0 is the root of the equation :

$$H^2u^*\left(\frac{1}{4\sin^2\frac{\pi H}{2(b-a)}} - \frac{1}{12} \right) = 1.$$

Proof : $J - h^2PU^* = J(I - J^{-1}h^2PU^*)$, where $U^* > \underline{0}$. J being monotone matrix, it is sufficient to prove that $I - J^{-1}h^2PU^*$ is monotone matrix. Proceeding as in Lemma 9, the lemma follows.

Lemma 18: Let $-\infty < u^* \leq 0$, and $h < \sqrt{\frac{12}{-u^*}}$. If $(J - h^2PU^*)^{-1} = (g_{nm})_{n,m=1}^{N-1}$, then

$$g_{nm} = \begin{cases} \dfrac{1}{1+\frac{h^2u^*}{12}} \dfrac{\sinh(n\theta).\sinh(N-m)\theta}{\sinh(N\theta).\sinh(\theta)}, & n \leq m; \\[2ex] \dfrac{1}{1+\frac{h^2u^*}{12}} \dfrac{\sinh(m\theta).\sinh(N-n)\theta}{\sinh(N\theta).\sinh(\theta)}, & n \geq m; \end{cases}$$

where $\sinh(\theta/2) = \frac{h}{2}\sqrt{\frac{-u^*}{1+\frac{h^2u^*}{12}}}$.

Proof : By Lemma 16, $J - h^2PU^*$ is monotone matrix, for $h < \sqrt{\frac{12}{-u^*}}$. So it is invertible and $(J - h^2PU^*)^{-1} \geq 0$, by Theorem 2. Multiplying the n-th row of $(J - h^2PU^*)$ with the m-th column of $(J - h^2PU^*)^{-1}$, we get

$$(12) \quad \left(-1 - \frac{h^2u^*}{12}\right)g_{n-1,m} + \left(2 - \frac{10}{12}h^2u^*\right)g_{n,m} + \left(-1 - \frac{h^2u^*}{12} \right)g_{n+1,m}$$

$$= \begin{cases} 0, & \text{for } 1 \le n \le m-1 \\ 1, & \text{for } n = m \\ 0, & \text{for } m+1 \le n \le N-1 \end{cases} \quad ; \quad \text{where}$$

(13) $$g_{0,m} = g_{N,m} = 0.$$

The characteristic equation for (12) is given by

(14) $$(-1 - \frac{h^2u^*}{12})\xi^2 + (2 - \frac{10\ h^2u^*}{12})\xi + (-1 - \frac{h^2u^*}{12}) = 0.$$

If ξ_1 and ξ_2 are the two roots of (14), then

$$\xi_1 = \frac{a+b}{c} \quad \text{and} \quad \xi_2 = \frac{a-b}{c}, \text{ where}$$

$$a = -\left(2 - \frac{10}{12}h^2u^*\right),\ b = h\left(\frac{2}{3}\ h^2u^{*2} - 4u^*\right)^{1/2},\ c = 2\left(-1 - \frac{h^2u^*}{12}\right).$$

Since $\xi_1 . \xi_2 = 1$, we can set $\xi_1 = e^{\theta}$, and $\xi_2 = e^{-\theta}$. Then,

$$1 + 2\sinh^2(\theta/2) = \cosh(\theta) = \frac{e^{\theta} + e^{-\theta}}{2} = \frac{\xi_1 + \xi_2}{2} = \frac{a}{c}.$$

So, $$\sinh(\theta/2) = \sqrt{\frac{a-c}{2c}} = \frac{h}{2}\sqrt{\frac{-u^*}{1 + \frac{h^2u^*}{12}}}.$$

Since, ξ_1 and ξ_2 are the two distinct roots of the equation (14),

$$g_{nm} = R\ e^{n\theta} + S\ e^{-n\theta}.$$

Let us assume,

(15) $$g_{nm} = \begin{cases} R_1\ e^{n\theta} + S_1\ e^{-n\theta}, & n \le m \\ R_2\ e^{n\theta} + S_2\ e^{-n\theta}, & n \ge m \end{cases}$$

where R_1, S_1, R_2, S_2 are functions of m only. Using the condition (13), we get,

(16) $$S_1 = -R_1, \text{ and } S_2 = -R_2e^{2N\theta},$$

where R_1 and R_2 are the constants which are to determined such tha the definitions of g_{nm} given in (15) are consistent for $n = m$ an such that the middle condition of (12) holds. Then

(17) $$R_2 = \frac{R_1(e^{m\theta} - e^{-m\theta})}{e^{m\theta} - e^{(2N-m)\theta}},$$

and

(18) $$R_1 = \frac{1}{1+\frac{h^2u^*}{12}} \frac{\sinh(N-m)\theta}{2\sinh(N\theta).\sinh(\theta)}.$$

Using (16), (17), and (18) in (15) the lemma follows.

<u>Lemma 19</u>: Let $0 < u^* < \pi^2/(b-a)^2$, and $h < h_0$, where h_0 is the roo of the equation :

$$H^2u^*\left(\frac{1}{4\sin^2\frac{\pi H}{2(b-a)}} - \frac{1}{12} \right) = 1.$$

If $(J - h^2PU^*)^{-1} = (g_{nm})_{n,m=1}^{N-1}$, then

$$g_{nm} = \begin{cases} \dfrac{1}{1+\frac{h^2u^*}{12}} \dfrac{\sin(n\theta)}{\sin(N\theta)} \dfrac{\sin(N-m)\theta}{\sin(\theta)}, & n \le m \\ \dfrac{1}{1+\frac{h^2u^*}{12}} \dfrac{\sin(m\theta)}{\sin(N\theta)} \dfrac{\sin(N-n)\theta}{\sin(\theta)}, & n \ge m; \end{cases}$$

where $\sin(\theta/2) = \frac{h}{2}\sqrt{\dfrac{u^*}{1+\frac{h^2u^*}{12}}}$.

<u>Proof</u> : By Lemma 17, $J - h^2PU^*$ is monotone matrix, for all h h_0, so it is invertible and $(J - h^2PU^*)^{-1} \ge 0$, by Theorem 2. A in Lemma 18, multiplying the n-th row of $(J - h^2PU^*)$ with the m-t

column of $(J - h^2PU^*)^{-1}$, we get the equation

$$(19)\qquad (-1 - \frac{h^2u^*}{12})g_{n-1,m} + (2 - \frac{10}{12}h^2u^*)g_{n,m} + (-1 - \frac{h^2u^*}{12})g_{n+1,m}$$

$$= \begin{cases} 0, & \text{for } 1 \le n \le m-1 \\ 1, & \text{for } n = m \\ 0, & \text{for } m+1 \le n \le N-1 \end{cases} \quad ;\text{ where}$$

$$(20)\qquad g_{0,m} = g_{N,m} = 0,$$

the characteristic equation of which is given by

$$(21)\qquad (-1 - \frac{h^2u^*}{12})\,\xi^2 + (2 - \frac{10}{12}h^2u^*)\,\xi + (-1 - \frac{h^2u^*}{12}) = 0\,.$$

If ξ_1 and ξ_2 are the two roots of (21), then since $\xi_1.\xi_2 = 1$, we can set

$$\xi_1 = e^{i\theta}, \text{ and } \xi_2 = e^{-i\theta}.$$

Now, $\quad 1 - 2\sin^2(\theta/2) = \cos\theta = \dfrac{e^{i\theta} + e^{-i\theta}}{2} = \dfrac{\xi_1 + \xi_2}{2} = \dfrac{a}{c}$,

where $a = -(2 - \frac{10}{12}h^2u^*)$, and $c = 2(-1 - \frac{h^2u^*}{12})$.

So, $\quad \sin(\theta/2) = \sqrt{\dfrac{c-a}{2c}} = \dfrac{h}{2}\sqrt{\dfrac{u^*}{1 + \frac{h^2u^*}{12}}}.$

Since ξ_1, ξ_2 are distinct roots of the equation (21), we can write

$$(22)\qquad g_{nm} = \begin{cases} R_1\, e^{in\theta} + S_1\, e^{-in\theta}, & n \le m, \\ R_2\, e^{in\theta} + S_2\, e^{-in\theta}, & n \ge m, \end{cases}$$

R_1, S_1, R_2, S_2 being functions of m only. Using (20), we get,

$$(23)\qquad S_1 = -R_1, \text{ and } S_2 = -R_2e^{2iN\theta},$$

where R_1 and R_2 are the constants which are to determined such that

the definitions of g_{nm} given in (22) are consistent for $n = m$ and such that the middle condition of (19) holds. Then

(24) $$R_2 = \frac{R_1(e^{im\theta} - e^{-im\theta})}{e^{im\theta} - e^{i(2N-m)\theta}},$$

and

(25) $$R_1 = \frac{1}{1+\frac{h^2u^*}{12}} \, \frac{\sin(N-m)\theta}{2\sin(N\theta).\sin(\theta)}.$$

Using (23),(24), and (25) in (22) the result follows.

3.5 Convergence Analysis

Definition 14: Discretization error, at a point $x = x_n$, is the quantity $e_n = y_n - y(x_n)$, where y_n is the exact solution of the finite difference scheme for solving the BVP (1), calculated without round-off error, and $y(x)$ is the exact solution of the BVP.

Theorem 5: Let

$$\sum_{i=0}^{2} \alpha_i \, y_{n-1+i} - h^2 \sum_{i=0}^{2} \beta_i \, f_{n-1+i} = 0 \; ; \quad 1 \le n \le N-1$$

be the usual Cowell's method with function evaluation at three points, for solving a BVP (1), and

$$\sum_{i=0}^{2} \alpha_i \, y_{n-1+i} - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} \, f_{n-1+i} = 0 \; ; \quad 1 \le n \le N-1$$

be the corresponding β-optimal method in a Hilbert space, H. Then in a Hilbert space, H, in which D_x^6, the representer of 6-th derivative evaluation functional at x, exists and is uniformly bounded on [a,b], the β-optimal method is convergent.

Proof : Let

$$L\,[y(x);h] \equiv \sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) + h^2 \sum_{i=0}^{2} \beta_i y''(x_{n-1+i})$$

and

$$\hat{L}\,[y(x);h] \equiv \sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) + h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} y''(x_{n-1+i})$$

be the difference operators associated with the above usual and the β-optimal difference equations respectively, for solving the BVP (1). Let

(26) $$\|y''\| = \max_{a \le x \le b} |\, y''(x)\, |.$$

Then in a Hilbert space, H, in which D_x^6, the representer of 6-th derivative evaluation functional at x, exists and is uniformly bounded on [a,b], by Lemma 4, and using (26), we get

$$\begin{aligned}
|\,\hat{L}\,[y(x);h] - L\,[y(x);h]\,| &= h^2 \Big| \sum_{i=0} (\hat{\beta}_{i,n} - \beta_i) y''(x_{n-1+i}) \Big| \\
&\le h^2 \sum_{i=0}^{2} |(\hat{\beta}_{i,n} - \beta_i)|\; |y''(x_{n-1+i})| \\
&\le h^2 \|y''\| \sum_{i=0}^{2} |(\hat{\beta}_{i,n} - \beta_i)| \\
&\le h^2 \|y''\|\, O(h^2) = O(h^4).
\end{aligned}$$

Hence, $|\hat{L}\,[y(x);h]| - |L\,[y(x),h]| = O(h^4).$

Since $L[y(x);h]$ is consistent, $|\, L[y(x);h]\, | = o(h^2) = h^2\delta(h)$, where $\delta(h) \longrightarrow 0$, as $h \longrightarrow 0$, so,

$|\hat{L}\,[y(x);h]| \le |L\,[y(x),h]| + O(h^4) = o(h^2) + O(h^4) = o(h^2)$, so,

(27) $$|\ \hat{L}\ [y(x);h]\ | = h^2\delta(h).$$

It follows that we can write

(28) $$\sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} f(x_{n-1+i}, y(x_{n-1+i})) = \chi_n h^2 \delta(h),$$

where χ_n is some constant, for $1 \le n \le N-1$, and $X = \max\limits_{a \le x \le b} |\chi_n|$.

Whereas the optimal method for y_n, is given by,

(29) $$\sum_{i=0}^{2} \alpha_i y_{n-1+i} - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} f(x_{n-1+i}, y_{n-1+i}) = 0.$$

Let $e_n = y_n - y(x_n)$, $1 \le n \le N-1$, where $e_0 = e_N = 0$,

and $u_n = \frac{\partial}{\partial y} f(x_n, y_n + \xi_n e_n)$, where $0 < \xi_n < 1$; $1 \le n \le N-1$.

Subtracting (29) from (28), we get the error equation:

(30) $$\sum_{i=0}^{2} \alpha_i e_{n-1+i} - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} u_{n-1+i} e_{n-1+i} = \chi_n h^2 \delta(h),\ 1 \le n \le N-1.$$

In matrix notation,

$$(J - h^2 \hat{P} U)\ e = \hat{X} h^2 \delta(h),$$

so that

(31) $$e = (J - h^2 \hat{P} U)^{-1} \hat{X} h^2 \delta(h),$$

where J, $\hat{P}$, U and U^* are defined in the Definitions 4,6,7 and 9,

$e = [e_1, e_2, \ldots\ldots, e_{N-1}]^T$ and $\hat{X} = [\chi_1, \chi_2, \ldots\ldots\ldots, \chi_{N-1}]^T$.

Since, $U \le U^*$ and $\hat{P} \ge \underline{0}$, we have

(32) $$J - h^2 \hat{P} U \ge J - h^2 \hat{P} U^*.$$

<u>Case 1</u>: $-\infty < u^* \le 0$

Then $$J - h^2 \hat{P} U \ge J - h^2 \hat{P} U^* \ge J.$$

Now, by Lemma 8, $J - h^2\hat{P}U$ is monotone matrix for all $h < \sqrt{\frac{6}{-u_*}}$, provided $\Phi h^2 \le \frac{1}{12}$. J is also a monotone matrix. Hence by Theorem 4, $(J - h^2\hat{P}U)^{-1} \le J^{-1}$. As in Henrici([96], p. 363),

$$(J^{-1})_{n,m} = \begin{cases} \dfrac{(N-n)m}{N}, & n \le m \\ \dfrac{n(N-m)}{N}, & n \ge m \end{cases}$$

and
$$\| J^{-1} \|_\infty = \frac{N^2}{8}$$

from (31),
$$| e | \le J^{-1} | \hat{X} | h^2 \delta(h),$$

where $|v|$ for a vector $v = (v_1, v_2, \ldots, v_n)^T$ is defined by

$$| v | = (|v_1|, |v_2|, \ldots, |v_n|)^T.$$

So,
$$\| e \|_\infty \le \| J^{-1} \|_\infty \| \hat{X} \|_\infty h^2 \delta(h).$$

Hence, $| e_n | \le \| e \|_\infty \le \frac{N^2}{8} X h^2 \delta(h) = \frac{(b-a)^2}{8} X \delta(h), \quad 1 \le n \le N-1.$

So, $e_n \longrightarrow 0$, as $h \longrightarrow 0$. Hence the convergence.

<u>Case 2</u> : $0 < u^* < \pi^2/(b-a)^2$

Then $U^* > \underline{0}$. By Lemma 9 and 13, $J - h^2\hat{P}U$ and $J - h^2\hat{P}U^*$ are monotone matrices for all $h < H_5$ where $H_5 \le \min\{h_1, h_2\}$;

where $h_1 = \sqrt{\frac{6}{-u_*}}$, provided $\Phi h^2 \le \frac{1}{12}$ and h_2 is the smallest root of the equation:

$$H^2 u^* \left[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2) 4\sin^2 \frac{\pi H}{2(b-a)} \right] - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

So, by Theorem 4, $\quad (J - h^2\hat{P}U)^{-1} \le (J - h^2\hat{P}U^*)^{-1}.$

Hence, from (31), $\quad | e | \le (J - h^2\hat{P}U^*)^{-1} | \hat{X} | h^2 \delta(h).$

So, $$\| e \|_\infty \le \| (J - h^2\hat{P}U^*)^{-1} \|_\infty \| \hat{X} \|_\infty h^2\delta(h).$$

Now, as in Theorem 11, established in section 3.7, we have

$$(J - h^2\hat{P}U^*)^{-1} = [\ I - (J - h^2PU^*)^{-1}\hat{\phi}h^4U^*\ ]^{-1}\ (J - h^2PU^*)^{-1},$$

where $\hat{\phi}$ is given by Definition 12. It follows that

$$\|(J - h^2\hat{P}U^*)^{-1}\|_\infty \le \|\ [I - (J - h^2PU^*)^{-1}\hat{\phi}\ h^4U^*]^{-1}\|_\infty\ \|(J - h^2PU^*)^{-1}\|_\infty$$

$$\le d_1\ d_2, \quad \text{say,}$$

where $$d_1 = \cfrac{1}{1 - \cfrac{\Phi h^2u^*}{1+\cfrac{h^2u^*}{12}}\ \cfrac{(b-a)^2}{8}\ \cfrac{N\theta}{\sin(N\theta)}\ \cfrac{\theta}{\sin\theta}} = O(1)$$

and $$d_2 = \cfrac{1}{1+\cfrac{h^2u^*}{12}}\ \frac{N^2}{8}\ \frac{N\theta}{\sin(N\theta)}\ \frac{\theta}{\sin\theta} = O(h^{-2})$$

which are obtained latter in Theorem 11. So

$$|\ e_n| \le \|\ e\ \|_\infty \le d_1d_2Xh^2\delta(h) = X\delta(h), \qquad 1 \le n \le N-1.$$

So, $e_n \longrightarrow 0$, as $h \longrightarrow 0$. Hence the convergence.

<u>Theorem 6</u> : Let

$$-\ y_{n-1} + 2y_n - y_{n+1} - h^2\ f_n = 0, \quad 1 \le n \le N-1$$

be Stormer's method for solving a boundary value problem (1) and

$$y_{n-1} + 2y_n - y_{n+1} - h^2\ \hat{\beta}_{1,n}\ f_n = 0, \quad 1 \le n \le N-1$$

be the corresponding optimal method where $\hat{\beta}_{1,n}$; $1 \le n \le N-1$ are the optimal coefficients. Then in a Hilbert space, H, in which D_x^4, the representer of 4-th derivative evaluation functional at x exists and is uniformly bounded on [a,b], the optimal method is convergent.

Proof : Let

$$L\,[y(x);h] \equiv \sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) + h^2 y''(x_n)$$

and

$$\hat{L}\,[y(x);h] \equiv \sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) + h^2\, \hat{\beta}_{1,n} y''(x_n)$$

be the difference operators associated with the above usual and the β-optimal difference equations for solving the BVP (1). Let

$$\| y'' \| = \max_{a \le x \le b} | y''(x) |.$$

Then as in Theorem 5, and using Lemma 4,

$$| \hat{L}\,[y(x);h] - L\,[y(x),h] | = h^2 | (\hat{\beta}_{1,n} - 1) y''(x_n) |$$

$$\le h^2 \| y''(x) \| \, |(\hat{\beta}_{1,n} - 1)| = O(h^4).$$

So, $\quad | \hat{L}\,[y(x);\, h] | - | L\,[y(x),h] | = O(h^4).$

Since $L\,[y(x);h]$ is consistent, $|L[y(x);h]| = o(h^2) = h^2\delta(h)$, where $\delta(h) \longrightarrow 0$, as $h \longrightarrow 0$, so,

$$| \hat{L}\,[y(x);h] | \le | L\,[y(x),h] | + O(h^4) = o(h^2) + O(h^4) = o(h^2).$$

Then, proceeding as in Theorem 5, and with notations therein we get the matrix equation

$$e = (J - h^2\hat{D}U)^{-1}\hat{X}h^2\delta(h). \tag{33}$$

Since, $U \le U^*$ and $\hat{D} > 0$, we have

$$J - h^2\hat{D}U \ge J - h^2\hat{D}U^*. \tag{34}$$

Case 1: $\quad -\infty < u^* \le 0.$

Then $\quad J - h^2\hat{D}U \ge J - h^2\hat{D}U^* \ge J\,.$

Now by Lemma 6, $J - h^2\hat{D}U$ is monotone matrix, for all h, provided $\Theta h^2 \le 1$. J is also a monotone matrix. Hence, by Theorem 4,

$$(J - h^2\hat{D}U)^{-1} \le J^{-1}.$$

Then as in the Case 1 of Theorem 5,

$$| e_n| \le \| e \|_\infty \le \frac{(b-a)^2}{8} X\delta(h); \qquad 1 \le n \le N-1.$$

So, $e_n \longrightarrow 0$, as $h \longrightarrow 0$. Hence the convergence.

Case 2 : $0 < u^* < \pi^2/(b-a)^2$.

Then $U^* > \underline{0}$. By Lemmas 7 and 11, $J - h^2\hat{D}U$ and $J - h^2\hat{D}U^*$ are monotone matrices for all $h < H_0$, provided $\Theta h^2 \le 1$, where H_0 is the smallest positive root of the equation :

$$H^2u^*(1 + \Theta H^2) - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

So, from (34), by Theorem 4, we get

$$(J - h^2\hat{D}U)^{-1} \le (J - h^2\hat{D}U^*)^{-1}.$$

Hence, from (33)

$$| e | \le (J - h^2\hat{D}U^*)^{-1}| \hat{X} |h^2\delta(h),$$

so that, $$\| e \|_\infty \le \| (J - h^2\hat{D}U^*)^{-1} \|_\infty \| \hat{X} \|_\infty h^2\delta(h).$$

Now, as in Theorem 10, to be established in section 3.7,

$$(J - h^2\hat{D}U^*)^{-1} = [I - (J - h^2U^*)^{-1}\hat{\theta}h^4U^*]^{-1}(J - h^2U^*)^{-1},$$

$$\|(J - h^2\hat{D}U^*)^{-1}\|_\infty \le \| [I - (J - h^2U^*)^{-1}\hat{\theta} h^4U^*]^{-1}\|_\infty \|(J - h^2U^*)^{-1}\|_\infty$$

$$\le c_1 c_2, \text{ say}$$

where $$c_1 = \frac{1}{1 - \Theta h^2u^*\frac{(b-a)^2}{8}\frac{N\theta}{\sin(N\theta)}\frac{\theta}{\sin\theta}} = O(1)$$

$$c_2 = \frac{N^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} = O(h^{-2}),$$

So, we get

$$|e_n| \le \| e \|_\infty \le c_1 c_2 X h^2 \delta(h) = X\delta(h), \quad 1 \le n \le N-1.$$

So, $e_n \longrightarrow 0$, as $h \longrightarrow 0$. Hence the convergence.

3.6 Newton's Method For Systems Of Nonlinear Equations

Let the n nonlinear equations

$$\phi_i(y_1, y_2, \ldots\ldots y_n) = 0, \qquad 1 \le i \le n,$$

for the n unknowns $y_1, y_2, \ldots, y_n$ be written in the vector form as,

(35) $$\phi(y) = 0.$$

Let $A(y)=(a_{ij}(y))_{i,j=1}^{n}$ denote the matrix with the elements given by

(36) $$a_{ij}(y) = \frac{\partial\phi_i(y)}{\partial y_j}.$$

Let the vector $y = y^{(0)}$ be an initial approximation to a solution of the system (35). Assuming $A(y^{(\nu)})$'s involved to be invertible, the successive better approximations $y^{(\nu)}$, $(\nu = 1,2,\ldots)$ are given by

(37) $$y^{(\nu+1)} = y^{(\nu)} - [A(y^{(\nu)})]^{-1} \phi(y^{(\nu)}), \qquad \nu = 0,1,2,\ldots..$$

constitute the Newton's method for the solutions of the system of nonlinear equations (35).

Now we state the following important theorem due to Kantorovich (Theorem 7.6, Henrici [96]).

Theorem 7: Assume that the following conditions are satisfied:

(i) For $y = y^{(0)}$, the initial approximation, the matrix $A(y^{(0)})$ has an inverse $\Gamma_0 = [A(y^{(0)})]^{-1}$ and an estimate for its norm is known,

(38) $$\| \Gamma_0 \| \le B_0,$$

(ii) The vector $\bar{y}^{(0)}$ approximately satisfies the system of equations (35) in the sense that

(39) $$\| \Gamma_0 \phi(y^{(0)}) \| \le \eta_0,$$

(iii) In the region defined by the inequality (42) below, the components of the vector $\phi(y)$ are twice differentiable with respect to the components of y and satisfy

(40) $$\sum_{j,k=1}^{n} \left| \frac{\partial^2 \phi_i(y)}{\partial y_j \partial y_k} \right| \le K, \qquad 1 \le i \le n$$

(iv) The constants B_0, η_0, K introduced above satisfy the inequality

(41) $$h_0 = B_0 \eta_0 K \le \frac{1}{2}.$$

Then the system of equations (35) has a solution y^* which is located in the cube

(42) $$\| y - y^{(0)} \| \le N(h_0)\eta_0 = \frac{1 - \sqrt{1-2h_0}}{h_0} \eta_0.$$

Moreover, the successive approximations $y^{(\nu)}$ defined by (37) existand converge to y^*, and the speed of convergence may be estimated by the inequality

(43) $$\| y^{(\nu)} - y^* \| \le \frac{1}{2^{\nu-1}} (2h_0)^{2^{\nu}-1} \eta_0, \qquad \nu = 0,1,2,\ldots .$$

Let us now study the convergence of Newton's Method for the system of nonlinear difference equations with optimal β-coefficients. Let

$$\hat{r}(y) \equiv Jy - h^2\hat{M}f(y) - \hat{a} = \underline{0} \tag{44}$$

be the system of nonlinear difference equations with optimal β-coefficients corresponding to the system with usual coefficients,

$$r(y) \equiv Jy - h^2Mf(y) - a = 0, \tag{45}$$

where $\hat{M} = \hat{D}$, when $M = I$ in the case of Stormer's method (4), with

$$\hat{a} = [A, 0, \ldots\ldots, 0, B]^T = a,$$

and $\hat{M} = \hat{P}$, when $M = P$ in the case of Cowell's method (5), with

$$\hat{a} = [A - \hat{\beta}_{0,1}h^2f(x_0, A), 0, \ldots\ldots\ldots, 0, B - \hat{\beta}_{2,N-1}h^2f(x_N, B)]^T,$$

$$a = [A - \beta_{0,1}h^2f(x_0, A), 0, \ldots\ldots\ldots, 0, B - \beta_{2,N-1}h^2f(x_N, B)]^T,$$

$$f(y) = [f(x_1, y_1), f(x_2, y_2), \ldots\ldots\ldots, f(x_{N-1}, y_{N-1})]^T.$$

The linearized system (44) then reads

$$\hat{r}\,(y^{(0)}) + [J - h^2\hat{B}F(y^{(0)})]\Delta y = 0, \tag{46}$$

where $F(y) = \mathrm{diag}\,\{f_y(x_1, y_1), f_y(x_2, y_2), \quad , f_y(x_{N-1}, y_{N-1})\}$

$y^{(0)}$ being an initial approximation to a solution of the system (35), we get

$$\hat{r}\,(y^{(0)}) + \hat{A}(y^{(0)})\Delta y = 0,$$

where $$\hat{A}(y) = J - h^2\,\hat{B}\,F(y).$$

Its solution is given by

$$\Delta y = \Delta y^{(0)} = -\,[\hat{A}(y^{(0)})]^{-1}\,\hat{r}(y^{(0)}),$$

which implies, $y^{(1)} = y^{(0)} - [\hat{A}(y^{(0)})]^{-1}\,\hat{r}(y^{(0)})$.

To prove the uniqueness of the solution of (44), for solving the BVP (1), suppose, if possible, y and z are any two solutions of (44), then we can write

$$f(x_n, z_n) - f(x_n, y_n) = u_n(z_n - y_n),$$

where u_n is a value of $\frac{\partial f}{\partial y}$.

Let $d_n = z_n - y_n$, $1 \le n \le N-1$, $d = [d_1, d_2, \ldots, d_{N-1}]^T$ and $U = [u_1, u_2, \ldots, u_{N-1}]^T$, which is given by Definition 7. Then from the system of equations (44) we get an equation for d,

$$[J - h^2\hat{M}U]d = \underline{0}. \tag{47}$$

If $[J - h^2\hat{M}U]^{-1}$ is a nonsingular matrix, then $d = \underline{0}$ and $y = z$.

Now, we shall verify that under certain hypotheses, the conditions of Theorem 7 are satisfied for the system (44) with $\phi(y) = \hat{r}(y)$ and the solution of (44) is unique.

Firstly, we shall consider the situation, when $\hat{M} = \hat{P}$ in (44). If $\hat{r}(y) = [\hat{r}_1(y), \hat{r}_2(y), \ldots, \hat{r}_{N-1}(y)]^T$,

then $\phi_n(y) = \hat{r}_n(y) = - y_{n-1} + 2y_n - y_{n+1}$

$$+ h^2\{ \hat{\beta}_{0n} f(x_{n-1}, y_{n-1}) + \hat{\beta}_{1n} f(x_n, y_n) + \hat{\beta}_{2n} f(x_{n+1}, y_{n+1})\}.$$

Let $L_2 = \max\limits_{\substack{a \le x \le b \\ -\infty < y < \infty \\ 1 \le i,\, j \le N-1}} \left| \frac{\partial^2}{\partial y_i \partial y_j} f(x,y) \right|$, then

using Corollary 3, and the fact that $\beta_0 + \beta_1 + \beta_2 = \frac{1}{12} + \frac{10}{12} + \frac{1}{12} = 1$,

$$\sum_{l,m=1}^{N-1} \left| \frac{\partial^2 \phi_n(y)}{\partial y_l \partial y_m} \right| \le h^2 L_2(\hat{\beta}_{0n} + \hat{\beta}_{1n} + \hat{\beta}_{2n}) \le h^2 L_2(1 + 3\Phi h^2) \le \frac{5}{4} h^2 L_2 ,$$

provided that $\Phi h^2 \le \frac{1}{12}$.

Hence the condition (iii) of Theorem 7, is satisfied with

$$K = \frac{5}{4} h^2 L_2. \tag{48}$$

Let the initial approximations $y^{(0)}$ be defined by

$$y_n^{(0)} = z(x_n), \qquad 1 \le n \le N-1.$$

Let

$$\tilde{R} = \max_{1 \le n \le N-1} \left| \frac{1}{h^2} \left\{ \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} f(x_{n-1+i}, z(x_{n-1+i})) \right\} \right|. \tag{49}$$

If $\hat{r}(y^{(0)}) = \left(\hat{r}_1(y^{(0)}), \hat{r}_2(y^{(0)}), \ldots, \hat{r}_{N-1}(y^{(0)}) \right)^T$,

then for $1 \le n \le N-1$,

$$|\hat{r}_n(y^{(0)})| = \left| \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} f(x_{n-1+i}, z(x_{n-1+i})) \right| \le h^2 \tilde{R}.$$

So, $\quad \| \Gamma_0 \hat{r}(y^{(0)}) \| \le \| \Gamma_0 \| \, \| \hat{r}(y^{(0)}) \| \le B_0 h^2 \tilde{R}.$

Hence, the condition (ii) of Theorem 7, holds with

$$\eta_0 = B_0 h^2 \tilde{R}. \tag{50}$$

Let $u_* = \inf\limits_{\substack{a \le X \le b \\ 1 \le i,\, j \le N-1}} \frac{\partial f_i}{\partial y_j}$, $\quad u^* = \sup\limits_{\substack{a \le X \le b \\ 1 \le i,\, j \le N-1}} \frac{\partial f_i}{\partial y_j}$, $\quad U_* = u^* I$, $\quad U^* = u_* I$.

Then, $\quad \hat{A}(y) = J - h^2 \hat{P} F(y) \ge J - h^2 \hat{P} U^*$.

<u>Case 1:</u> $\quad -\infty < u^* \le 0$

Then $U^* \le \underline{0}$. Since $F(y^{(0)}) \le U^* \le \underline{0}$,

$$\hat{A}(y^{(0)}) = J - h^2 \hat{P} F(y^{(0)}) \ge J - h^2 \hat{P} U^* \ge J.$$

Using Lemma 8, $J - h^2 \hat{P} F(y^{(0)})$ is monotone for all $h < h_1$, where

$h_1=\sqrt{\frac{6}{-u_*}}$, provided $\Phi h^2 \le 1/12$. J is also a monotone matrix. Hence by Theorem 4,

$$[\hat{A}(y^{(0)})]^{-1} \le J^{-1}.$$

Since, by Henrici [96], $\| J^{-1} \|_\infty \le \frac{N^2}{8} = \frac{(b-a)^2}{8h^2}$,

the condition (i) of Theorem 7, holds with

$$B_0 = \frac{(b-a)^2}{8h^2}. \tag{51}$$

By (50), $$\eta_0 = \frac{(b-a)^2}{8}\tilde{R}.$$

The condition (iv) of Theorem 7, which guarantees the convergence of Newton's process, thus turns out to be satisfied, if

$$h_0 = B_0\eta_0 K = \frac{(b-a)^2}{8h^2}\frac{(b-a)^2}{8}\tilde{R}\,\frac{5}{4}h^2L_2 \le \frac{1}{2},$$

i.e., if

$$\tilde{R} \le \frac{128}{5}\,\frac{1}{L_2(b-a)^4}. \tag{52}$$

Now by Lemma 8, $J - h^2\hat{P}U$ is a monotone matrix for all $h < h_1$, provided $\Phi h^2 \le \frac{1}{12}$ and hence is nonsingular, by Theorem 2. So, by (47), it follows that $d = \underline{0}$, which follows that the system of equations $Jy - h^2\hat{P}f(y) - \hat{a} = \underline{0}$ has unique solution.

<u>Case 2</u>: $0 < u^* < \pi^2/(b-a)^2$.

Then $U^* \ge \underline{0}$. Since $F(y^{(0)}) \le U^*$,

$$\hat{A}\,(y^{(0)}) = J - h^2\hat{P}F(y^{(0)}) \ge J - h^2\hat{P}U^*.$$

Using Lemma 9, $J - h^2\hat{P}F(y^{(0)})$ is monotone for all $h < \min\{h_1,h_2\}$, provided $\Phi h^2 \le \frac{1}{12}$, where $h_1 = \sqrt{\frac{6}{-u_*}}$, and h_2 is the smallest

positive root of the equation:

$$H^2u^*\left[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2)4\sin^2 \frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

So, by Theorem 4,

$$[\hat{A}(y^{(0)})]^{-1} \le [J - h^2\hat{P}U^*]^{-1}.$$

Then

$$(J - h^2\hat{P}U^*) = J - h^2(P + h^2\hat{\phi})U^* = (J - h^2PU^*) - h^4\hat{\phi}U^*,$$

where P and $\hat{\phi}$ are the matrices given by Definition 10, 12.

$$\text{So, } (J - h^2\hat{P}U^*)^{-1} = \left[(J - h^2PU^*)[I - (J - h^2PU^*)^{-1}\, h^4\hat{\phi}U^*]\right]^{-1}$$

$$= [I - (J - h^2PU^*)^{-1}\, h^4\hat{\phi}U^*]^{-1}(J - h^2PU^*)^{-1}.$$

So,

$$\|(J - h^2\hat{P}U^*)^{-1}\|_\infty \le \|\, [I - (J - h^2PU^*)^{-1}\hat{\phi}h^4U^*]^{-1}\|_\infty\, \|(J - h^2PU^*)^{-1}\|_\infty$$

$$\le d_1\, d_2, \text{ say},$$

where $$d_1 = \frac{1}{1 - \dfrac{\Phi h^2u^*}{1+\dfrac{h^2u^*}{12}}\,\dfrac{(b-a)^2}{8}\,\dfrac{N\theta}{\sin(N\theta)}\,\dfrac{\theta}{\sin\theta}} = O(1)$$

and $$d_2 = \frac{1}{1+\dfrac{h^2u^*}{12}}\,\frac{N^2}{8}\,\frac{N\theta}{\sin(N\theta)}\,\frac{\theta}{\sin\theta} = O(h^{-2}),$$

which are obtained in Theorem 11 in section 3.7. So, the condition (i) of Theorem 7 holds with

(53) $$B_0 = d_1d_2.$$

By (50), $$\eta_0 = d_1d_2h^2\tilde{R}.$$

Note that the required K, for the Kantorovich Theorem is given by (48). Hence, the condition (iv) of Theorem 7, which guarantees the

convergence of Newton's process, will be satisfied if

$$h_0 = B_0\eta_0 K = d_1^2 d_2^2 h^2 \tilde{R}\ \frac{5}{4}h^2 L_2 \le \frac{1}{2},$$

i.e., if

$$(54) \qquad \tilde{R} \le \frac{128}{5L_2(b-a)^4}\left[1+\frac{h^2u^*}{12}\right]^2\left[\frac{\sin(N\theta)}{N\theta}\ \frac{\sin\theta}{\theta} - \frac{\Phi h^2 u^*}{1+\frac{h^2u^*}{12}}\ \frac{(b-a)^2}{8}\right]^2.$$

Now by Lemma 9, $J - h^2\hat{P}U$ is a monotone matrix for all $h <$ min $\{h_1, h_2\}$, provided $\Phi h^2 \le \frac{1}{12}$, where h_1 and h_2 are as given earlier. Hence, it is nonsingular, by Theorem 2. So, by (47), it follows that the system of equations $Jy-h^2\hat{P}f(y)-\hat{a} = \underline{0}$ has unique solution.

Thus, we can state the following Theorem.

<u>Theorem 8</u> : Let $\hat{r}(y) \equiv Jy - h^2\ \hat{P}\ f(y) - \hat{a} = \underline{0}$, be the system of finite difference equations with optimal β- coefficients, arisen from a boundary value problem (1). Assume that $|\hat{\beta}_{in} - \beta_i| \le \Phi h^2$, for $i = 0,1,2$; $1 \le n \le N-1$, in a Hilbert space, H, in which D_x^6, the representer of 6-th derivative evaluation functional at x exists and is uniformly bounded in [a,b]. Let the initial approximation be given by $y_n^{(0)} = z(x_n)$, $1 \le n \le N-1$, and $\tilde{R}$ be defined by (49). If L_2 is an upper bound for $\frac{\partial^2 f(x,y)}{\partial y_i \partial y_j}$ in $a \le x \le b$, $-\infty < y < \infty$, $1 \le i, j \le N-1$, then the system (44) possesses a unique solution which can be obtained by Newton's method, if $\tilde{R}$ satisfies (52), in case of $-\infty < u^* \le 0$, for all $h < h_1$, and (54), in case of $0 < u^* < \pi^2/(b-a)^2$, for all $h <$ min (h_1, h_2), where $h_1 = \sqrt{\frac{6}{-u_*}}$, and h_2 is the smallest positive root of the equation :

$$H^2u^*\left[(1+3\Phi H^2) - (\frac{1}{12}+\Phi H^2)4\sin^2\frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

provided $\Phi h^2 \le 1/12$.

Following the proof of the convergence of Newton's method in the usual case, as given in Henrici [96], let the initial approximations $y^{(0)}$ be defined by

$$y_n^{(0)} = z\,(x_n), \qquad 1 \le n \le N-1, \tag{55}$$

where $z(x)$ is a p+2 times differentiable function satisfying $z(a) = A$, $z(b) = B$; p being the order of the difference operator.

Let

$$Z = \max_{a \le x \le b} |\ z^{(p+2)}(x)\ |$$

and

$$R = \max_{a \le x \le b} |\ z''(x) + f(x, z(x))\ |. \tag{56}$$

Let $L[y(x);h]$ and $\hat{L}[y(x);h]$ be the difference operators associated with the Cowell's usual method (5) and the corresponding β-optimal method (6) for solving the BVP (1).

Let $$\|\ y''\ \| = \max_{a \le x \le b} |\ y''\ (x)\ |.$$

Then

$$|\hat{L}\ [z(x);h]| = |\sum_{i=0}^{2} \alpha_i z(x+(i-1)h) + h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} z''(x+(i-1)h)| = O(h^4).$$

Now, for $1 \le n \le N-1$

$$|\ \hat{r}_n(y^{(0)})| = \left| \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n}\ f(x_{n-1+i}\ , z(x_{n-1+i})) \right|$$

$$\le \left| \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} z''(x_{n-1+i}) \right|$$

$$+ h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n}\ |\ z''(x_{n-1+i}) + f(x_{n-1+i},\ z(x_{n-1+i}))|$$

$$\leq |\hat{L}\ [z(x_n); h]| + h^2R(\hat{\beta}_{0n} + \hat{\beta}_{1n} + \hat{\beta}_{2n}).$$

Since the order of $L[y(x); h]$ is $p=4$, using Lemma 3 and Corollary 3, we get

$$|\ \hat{r}_n(y^{(0)})| \leq G^*Zh^6 + h^2R(1 + 3\Phi h^2) \leq G^*Zh^6 + \tfrac{5}{4}h^2R,$$

provided that $\Phi h^2 \leq \frac{1}{12}$.

So, $\quad \| \Gamma_0\hat{r}(y^{(0)}) \| \leq \| \Gamma_0\| \ \| \hat{r}(y^{(0)}) \| \leq B_0\left(G^*Zh^6 + \tfrac{5}{4}h^2R\right).$

Hence, the condition (ii) of Theorem 7, holds with

$$\eta_0 = B_0\left(G^*Zh^6 + \tfrac{5}{4}h^2R\right), \tag{57}$$

with K as in the previous theorem, given by (48).

<u>Case 1:</u> $\quad -\infty < u^* \leq 0.$

Let B_0 be as in the Case 1 of the previous Theorem, given by (51). Using (57) for η_0, the condition (iv) of Theorem 7 is satisfied if

$$h_0 = B_0\eta_0K \leq \frac{1}{2},$$

i.e., if $\quad h_0 = \dfrac{(b-a)^2}{8h^2}\ \dfrac{(b-a)^2}{8}\ \left(G^*Zh^4 + \tfrac{5}{4}R\right)\tfrac{5}{4}h^2L_2 \leq \dfrac{1}{2},$

i.e., if

$$\left(G^*Zh^4 + \tfrac{5}{4}R\right) \leq \frac{128}{5}\ \frac{1}{L_2(b-a)^4}. \tag{58}$$

The uniqueness of the solution of (44) holds for $h < h_1$, as in the Case 1 of the previous theorem, provided $\Phi h^2 \leq \frac{1}{12}$.

<u>Case 2:</u> $\quad 0 < u^* < \pi^2/(b-a)^2.$

With B_0 as in the Case 2 of the previous Theorem given by (53), using (57) for η_0, the condition (iv) of Theorem 7 is satisfied, if

$$h_0 = B_0\eta_0K = d_1^2d_2^2\ \left(G^*Zh^6 + \tfrac{5}{4}h^2R\right)\ \tfrac{5}{4}h^2L_2 \leq \tfrac{1}{2}, \qquad \text{i.e., if}$$

$$(59)\qquad \left(G^{*}Zh^{4} + \frac{5}{4}R\right) \le$$

$$\frac{128}{5L_2(b-a)^4}\left[1 + \frac{h^2u^*}{12}\right]^2 \left[\frac{\sin(N\theta)}{N\theta}\,\frac{\sin\theta}{\theta} - \frac{\Phi h^2 u^*}{1+\frac{h^2u^*}{12}}\,\frac{(b-a)^2}{8}\right]^2.$$

The uniqueness of the solution of (44) holds for $h < \min\{h_1, h_2\}$, as in the Case 2 of the previous theorem, provided $\Phi h^2 \le \frac{1}{12}$.

Thus we get the following corollary.

<u>Corollary 5:</u> Let the system of finite difference equations (44) correspond to a BVP (1). If p denotes the order of the difference operator $L[y(x);h]$ associated with the usual method (5), assume that the exact solution $y(x)$ has a continuous (p+2)-nd derivative in $[a,b]$ and let

$$Z = \max_{a\le x\le b} |\, y^{(p+2)}(x)\,|.$$

Let R be defined by (56) and the initial approximation be defined by (55) and L_2 is an upper bound for $\frac{\partial^2 f(x,y)}{\partial y_i\,\partial y_j}$ in $a \le x \le b$, $-\infty < y < \infty$, $1 \le i,j \le N-1$. Assume that $|\hat{\beta}_{in} - \beta_i| \le \Phi h^2$, for $i = 0,1,2$; $1 \le n \le N-1$, in a Hilbert space, H, in which D_x^6, the representer of 6-th derivative evaluation functional exists and is uniformly bounded in $[a,b]$. Then the system (44) possesses a unique solution which can be found by Newton's method, if h satisfies (58) in case of $-\infty < u^* \le 0$, with $h < h_1$, and (59) in case of $0 < u^* < \pi^2/(b-a)^2$, with $h < \min\{h_1, h_2\}$, where $h_1 = \sqrt{\frac{6}{-u_*}}$, and h_2 is the smallest positive root of the equation :

$$H^2u^*\left[(1 + 3\Phi H^2) - (\tfrac{1}{12} + \Phi H^2)4\sin^2\frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

provided that $\Phi h^2 \le 1/12$.

Secondly, we shall consider the situation, when $\hat{M} = \hat{D}$ in (44). Then we have the system of equations $\hat{r}(y) \equiv Jy - h^2\hat{D}f(y) - \hat{a} = \underline{0}$.

If $\quad \hat{r}(y) = [\hat{r}_1(y), \hat{r}_2(y), \ldots\ldots, \hat{r}_{N-1}(y)]^T$,

then $\quad \phi_n(y) \equiv \hat{r}_n(y) = - y_{n-1} + 2y_n - y_{n+1} + h^2\, \hat{\beta}_{1n}\, f(x_n, y_n)$.

Let
$$L_2 = \max_{\substack{a \le x \le b \\ -\infty < y < \infty}} \left| \frac{\partial^2}{\partial y_i \partial y_j} f(x,y) \right|.$$

Now using Corollary 4, and assuming that $\Theta h^2 \le 1$,

$$\sum_{l,m=1}^{N-1} \left| \frac{\partial^2 \phi_n(y)}{\partial\, y_l \partial\, y_m} \right| \le h^2 L_2\, \hat{\beta}_{1n} \le h^2 L_2 (1 + \Theta h^2) \le 2h^2 L_2.$$

Hence the condition (iii) of Theorem 7, is satisfied with

$$K = 2h^2 L_2. \tag{60}$$

Let the initial approximation $y^{(0)}$ be defined by

$$y^{(0)} = z(x_n), \qquad 1 \le n \le N-1, \quad \text{and}$$

$$\tilde{R} = \max_{1 \le n \le N-1} \left| \frac{1}{h^2} \left\{ \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2 \hat{\beta}_{1n} f(x_n, z(x_n)) \right\} \right|. \tag{61}$$

Then for $1 \le n \le N-1$,

$$\left| \hat{r}_n(y^{(0)}) \right| = \left| \sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2\, \hat{\beta}_{1n} f(x_n, z(x_n)) \right| \le h^2 \tilde{R}.$$

So, $\qquad \| \Gamma_0 \hat{r}_n(y^{(0)}) \| \le \| \Gamma_0 \| \, \| \hat{r}_n(y^{(0)}) \| \le B_0 h^2 \tilde{R}.$

Hence the condition (iii) of Theorem 7, holds with

$$\eta_0 = B_0 h^2 \tilde{R}. \tag{62}$$

<u>Case 1:</u> $\qquad -\infty < u^* \le 0.$

Then $U^* \le \underline{0}$. Since $F(y^{(0)}) \le U^*$,

$$\hat{A}(y^{(0)}) = J - h^2\hat{D}F(y^{(0)}) \geq J - h^2\hat{D}U^* \geq J.$$

By Lemma 6, $J- h^2\hat{D}F(y^{(0)})$ is monotone matrix for all h provided $\Theta h^2 \leq 1$. J is also a monotone matrix. So, by Theorem 2,

$$[J - h^2\hat{D}F(y^{(0)})]^{-1} \leq J^{-1}.$$

Proceeding as in the Case 1 of Theorem 8, we get,

(63) $$B_0 = \frac{(b-a)^2}{8h^2}.$$

By (62) and (63), $$\eta_0 = \frac{(b-a)^2}{8} \tilde{R}.$$

and K is given by (60). The condition (iv) of Theorem 7, which guarantees the convergence of Newton's process, thus turns out to be satisfied, if

$$h_0 = B_0\eta_0 K = \frac{(b-a)^2}{8h^2} \frac{(b-a)^2}{8} \tilde{R}2h^2L_2 \leq \frac{1}{2},$$

i.e., if

(64) $$\tilde{R} \leq \frac{16}{L_2(b-a)^4}.$$

By Lemma 6, $J- h^2\hat{D}U$ is a monotone matrix for all h, provided $\Theta h^2 \leq 1$. Hence by (47), the system of equations $Jy -h^2\hat{D}f(y) - \hat{a} = \underline{0}$ has unique solution.

Case 2: $0 < u^* < \pi^2/(b-a)^2$.

Then $U^* \geq \underline{0}$. Since $F(y^{(0)}) \leq U^*$,

$$\hat{A}(y^{(0)}) = J - h^2\hat{D}F(y^{(0)}) \geq J - h^2\hat{D}U^*.$$

By Lemma 7, $J - h^2\hat{D}F(y^{(0)})$ is a monotone matrix for all $h < H_0$, provided $\Theta h^2 \leq 1$, where H_0 is the smallest root of the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

So, by Theorem 4,

$$[\hat{A}\ (y^{(0)})]^{-1} \le [J - h^2\hat{D}U^*]^{-1}.$$

Now, $\quad (J - h^2\hat{D}U^*) = J - h^2(I + h^2\hat{\theta})U^* = (J - h^2U^*) - h^4\hat{\theta}U^*,$

where $\hat{\theta}$ is given in Definition 13, and by Corollary 4, $\|\ \hat{\theta}\ \| \le \Theta$.

So, $\quad (J - h^2\hat{D}U^*)^{-1} = \left[(J - h^2U^*)\ [I - (J - h^2U^*)^{-1}\ h^4\hat{\theta}U^*]\right]^{-1}$

$$= [I - (J - h^2U^*)^{-1}h^4\hat{\theta}U^*]^{-1}\ (J - h^2U^*)^{-1},$$

so that

$$\|(J - h^2\hat{D}U^*)^{-1}\|_\infty \le \|\ [I - (J - h^2DU^*)^{-1}\hat{\phi}\ h^4U^*]^{-1}\|_\infty\ \|(J - h^2DU^*)^{-1}\|_\infty$$

$$\le c_1\ c_2, \text{ say}$$

where $\quad c_1 = \dfrac{1}{1 - \Theta\ h^2u^*\ \dfrac{(b-a)^2}{8}\ \dfrac{N\theta}{\sin(N\theta)}\ \dfrac{\theta}{\sin\theta}} = O(1),$

$$c_2 = \frac{N^2}{8}\ \frac{N\theta}{\sin(N\theta)}\ \frac{\theta}{\sin\theta} = O(h^{-2}),$$

which are obtained in Theorem 10 in section 3.7. So, the condition (i) of Theorem 7, holds with

(65) $$B_0 = c_1\ c_2.$$

By (62) and (65), $\quad \eta_0 = c_1c_2h^2\tilde{R}.$

K is given by (60). Hence, the condition (iv) of Theorem 7, which guarantees convergence of Newton's process, will be satisfied, if

$$h_0 = B_0\eta_0K = c_1^2c_2^2h^2\tilde{R}2h^2L_2 \le \frac{1}{2},$$

i.e., if

$$\tilde{R} \le \frac{16}{L_2(b-a)^4}\left[\frac{\sin(N\theta)}{N\theta}\,\frac{\sin\theta}{\theta} - \Theta h^2 u^* \frac{(b-a)^2}{8}\right]^2. \tag{66}$$

By Lemma 7, $J - h^2\hat{D}U$ is a monotone matrix for all $h < H_0$, where H_0 is as given above, provided $\Theta h^2 \le 1$. Hence, by (47), the system of equations $Jy - h^2\hat{D}f(y) - \hat{a} = \underline{0}$ has unique solution.

Thus we can state the following theorem.

<u>Theorem 9</u> : Let $\hat{r}(y) \equiv Jy - h^2\,\hat{D}\,f(y) - \hat{a} = \underline{0}$ be the system of finite difference equations with optimal β coefficient, corresponding to usual Stormer's method (4), arisen from a BVP (1). Assume that $|\,\hat{\beta}_{in} - \beta_i| \le \Phi h^2$, for $i = 0,1,2;\ 1 \le n \le N-1$, in a Hilbert space, H, in which D^4_x, the representer of 4-th derivative evaluation functional at x exists and is uniformly bounded in [a,b]. Let the initial approximation be given by $y_n^{(0)} = z(x_n)$, $1 \le n \le N-1$, and let $\tilde{R}$ be defined by (61). If L_2 is an upper bound for $\frac{\partial^2 f(x,y)}{\partial y_i \partial y_j}$ in $a \le x \le b;\ -\infty < y < \infty;\ 1 \le i,j \le N-1$, then the above system possesses a unique solution which can be obtained by Newton's method, if $\tilde{R}$ satisfies (64) in the case of $-\infty < u^* \le 0$, and (66) in the case of $0 < u^* < \pi^2/(b-a)^2$, with $h < H_0$, where H_0 is the smallest positive root of the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

provided $\Theta h^2 \le 1$.

Let us now proceed as in Corollary 5. Let the initial approximation $y^{(0)}$ be defined by

$$y^{(0)} = z(x_n), \quad 1 \le n \le N-1,$$

where $z(x)$ is a $p+2 = 4$ times differentiable function satisfying $z(a) = A$, $z(b) = B$; p being the order of the difference operator $L[y(x);\ h]$ and let

$$Z = \max_{a \le x \le b} |z^{(4)}(x)|,$$

and

$$R = \max_{a \le x \le b} |z''(x) + f(x,z(x))|.$$

Let $L[y(x);\ h]$ and $\hat{L}[y(x);h]$ be the difference operators associated with Stormer's usual method (4) and the corresponding β-optimal method (10). Since $L[y(x);\ h]$ has order $p = 2$, by Lemma 3

$$|\ \hat{L}\ [z(x);\ h]\ | = |\ \sum_{i=0}^{2} \alpha_i z(x+(i-1)h) - h^2\ \hat{\beta}_{1,n} z''(x)\ | \le G^* Z h^4.$$

Now, for $1 \le n \le N-1$,

$$|\ \hat{r}_n(y^{(0)})\ | = |\sum_{i=0}^{2} \alpha_i z(x_{n-1+i}) - h^2\ \hat{\beta}_{1n} f(x_n, z(x_n))|$$

$$\le |\ \hat{L}\ [z(x_n);\ h]\ | + h^2 R \hat{\beta}_{1n}$$

$$\le G^* Z h^4 + h^2\ R(1 + \Theta h^2) \le G^* Z h^4 + 2h^2 R,$$

provided that $\Theta h^2 \le 1$. So,

$$\|\ \Gamma_0 \hat{r}(y^{(0)})\ \| \le \|\ \Gamma_0\ \|\ \|\ \hat{r}(y^{(0)})\ \| \le B_0\left(G^* Z h^4 + 2h^2 R\right).$$

Hence, the condition (ii) of Theorem 7, holds with

$$\eta_0 = B_0\left(G^* Z h^4 + 2h^2 R\right). \tag{67}$$

Let K be given by (60).

<u>Case 1:</u> $-\infty < u^* \le 0$.

With B_0 as in the Case 1 of Theorem 9, given by (63). From (67),

$$\eta_0 = \frac{(b-a)^2}{8h^2}\left(G^* Z h^4 + 2h^2 R\right).$$

The condition (iv) of Theorem 7, is satisfied, if

$$h_0 = B_0\eta_0 K = \frac{(b-a)^2}{8h^2}\,\frac{(b-a)^2}{8h^2}\left(G^*Zh^4 + 2h^2R\right)\,2h^2L_2 \le \frac{1}{2},$$

i.e., if

(68) $$\left(G^*Zh^2 + 2R\right) \le \frac{16}{L_2(b-a)^4}.$$

The uniqueness of the solution holds as in Case 1 of Theorem 9.

Case 2: $\quad 0 < u^* < \pi^2/(b-a)^2$.

B_0 is as in Case 2 of Theorem 9, given by (65). Then from (67)

$$\eta_0 = c_1c_2\left(G^*Zh^4 + 2h^2R\right).$$

The condition (iv) of Theorem 7, is satisfied, if

$$h_0 = B_0\eta_0 K = c_1^2c_2^2\left(G^*Zh^4 + 2h^2R\right)\,2h^2L_2 \le \frac{1}{2},$$

i.e., if

(69) $$\left(G^*Zh^4 + 2h^2R\right) \le \frac{16}{L_2(b-a)^4}\left[\frac{\sin(N\theta)}{N\theta}\,\frac{\sin\theta}{\theta} - \Theta h^2u^*\,\frac{(b-a)^2}{8}\right]^2.$$

The uniqueness of the solution follows as in Case 2 Theorem 9. Thus we get the following corollary.

Corollary 6: Let the system of finite difference equations $\hat{r}(y) \equiv Jy - h^2\hat{D}f(y) - \hat{a} = \underline{0}$ correspond to the BVP (1). Assume that the exact solution $y(x)$ has a continuous 4-th derivative in $[a,b]$ and let

$$Z = \max_{a\le x<b} |y^{(4)}(x)|.$$

Assume that $|\hat{\beta}_{1n} - 1| \le \Theta\, h^2$, for $1 \le n \le N-1$, in a Hilbert space, H, in which D_x^4, the representer of 4-th derivative evaluation functional exists and is uniformly bounded in $[a,b]$. If the initial approximation $y^{(0)}$ is defined by (55) and R is defined (56) and L_2

is an upper bound for $\frac{\partial^2 f(x,y)}{\partial y_i \partial y_j}$ in $a \le x \le b$, $-\infty \le y \le \infty$, $1 \le i,j \le N-1$, then the above system of equations possesses a unique solution, which can be found by Newton's method for all values of h, provided $\Theta h^2 \le 1$, satisfying (68) in the case of $-\infty < u^* \le 0$, and (69) in the case of $0 < u^* < \pi^2/(b-a)^2$, with $h < H_0$, where H_0 is the smallest possible root of the equation:

$$H^2 u^*(1 + \Theta H^2) - 4\sin^2 \frac{\pi H}{2(b-a)} = 0,$$

3.7 Stability Analysis

In this section, we shall establish stability theory for the β-optimal methods, corresponding to the usual Stormer's method (4) and the Cowell's method (5), and for those two usual methods adopted for solving a two point BVP (1). An important application of stability is in obtaining the error estimate which gives a relation between discretization error and local truncation error.

For solving an IVP or a BVP numerically, the set of discrete points $\{x_j\}$, employed on the given interval $[a,b]$, is called a net. We will take this net to be uniformly spaced, say

$$x_0 = a, \quad x_j = a + jh; \quad j = 1(1)N, \quad h = (b-a)/N.$$

The quantity h is called net spacing. A rule which assigns to each point x_j of the net a corresponding n vector v_j is called a net function, $\{v_j\}$.

__Theorem 10:__ Let $\hat{L}_1$ be the linear difference operator associated with the optimal method corresponding to the usual Stormer's method

(4) and a net function $\{v_i\}$ be defined as

$$\hat{L}_1 v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} - \hat{\beta}_{1,i} f(x_i, v_i) = 0; \qquad 1 \le i \le N-1,$$

where $\hat{\beta}_{1,i}$, $1 \le i \le N-1$ are the optimal coefficients corresponding to the usual coefficient $\beta_1 = 1$ and

$$|\hat{\beta}_{1,i} - 1| \le \Theta h^2, \qquad 1 \le i \le N-1.$$

Assume that $f(x,y)$ has continuous derivatives with respective to y, satisfying
$$u_* \le \frac{\partial f}{\partial y} \le u^*.$$

Then $\hat{L}_1$ is stable in the sense that for all net functions $\{v_i\}, \{w_i\}$

$$|v_i - w_i| \le M \left\{ \max\left(|v_0 - w_0|, \ |v_N - w_N| \right) + \max_{1 \le j \le N-1} |\hat{L}_1 v_j - \hat{L}_1 w_j| \right\},$$

for $1 \le i \le N-1$, for some constant M and some suitable restriction on h given in the following two cases.

<u>Case1 :</u> $\quad -\infty < u^* < 0$.

Then $\hat{L}_1$ is stable with $M = \hat{M}_1 = C_1 M_1$, where

$$\hat{M}_1 = \frac{1}{1 - \Theta h^2} \max\left\{1, \frac{1}{-u^*}\right\}, \quad \text{for all } h \text{ satisfying } \Theta h^2 < 1.$$

<u>Case 2:</u> $\quad 0 < u^* < \pi^2/(b-a)^2$.

Then $\hat{L}_1$ is stable with $M = \hat{M}_2 = C_2 M_2$, where

$$\hat{M}_2 = \frac{1}{1 - \Theta h^2 u^* \dfrac{(b-a)^2}{8} \dfrac{N\theta}{\sin(N\theta)} \dfrac{\theta}{\sin\theta}} \cdot \max\left\{ \frac{1}{\cos\frac{N\theta}{2}}, \ \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} \right\},$$

for all $h < \min\{H_1, H_2\}$, where H_1 is the smallest positive root of

the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2 \frac{\pi H}{2(b-a)} = 0,$$

and H_2 is the smallest positive root of the equation

$$H^2u^* - 4\sin^2 \frac{\pi H}{2(b-a)} = 0,$$

provided $\Theta h^2 < \min\left\{1 , \frac{8}{(b-a)^2u^*}\right\}$.

Proof: If $\{v_i\}$ and $\{w_i\}$ are any two net functions, then

$$h^2\hat{L}_1v_i = -(v_{i-1} - 2v_i + v_{i+1}) - h^2\hat{\beta}_{1,1}f(x_i,v_i),$$

$$h^2\hat{L}_1w_i = -(w_{i-1} - 2w_i + w_{i+1}) - h^2\hat{\beta}_{1,1}f(x_i,w_i).$$

So, $$h^2[\hat{L}_1v_i - \hat{L}_1w_i] = -(v_{i-1} - w_{i-1}) + 2(v_i-w_i) - (v_{i+1}-w_{i+1})$$
$$- h^2\hat{\beta}_{1,1}(v_i-w_i)\frac{\partial}{\partial y} f(x_i,w_i+\xi_i(v_i-w_i)).$$

Let $u_i = \frac{\partial}{\partial y} f(x_i,w_i+\xi_i(v_i-w_i)), \quad 1 \le i \le N-1.$

Then the above equation becomes

$$h^2[\hat{L}_1v_i - \hat{L}_1w_i] = -(v_{i-1}-w_{i-1}) + (2-h^2\hat{\beta}_{1,1}u_i)(v_i-w_i) - (v_{i+1}-w_{i+1});$$

for $1 \le i \le N-1$.

In matrix notation this system of equations becomes,

(70) $$(J - h^2\hat{D}U)[v - w] = b_1 + b_2,$$

where J, $\hat{D}$, U are $(N-1)\times(N-1)$ matrices given in Definitions 4,5, 7.

$[v - w] = [(v_1-w_1),(v_2-w_2),\ldots\ldots,(v_{N-1}-w_{N-1})]^T,$

$b_1 = [(v_0-w_0),0,\ldots\ldots,0,(v_N-w_N)]^T,$

$b_2 = h^2[(\hat{L}_1v_1-\hat{L}_1w_1),(\hat{L}_1v_2-\hat{L}_1w_2),\ldots\ldots,(\hat{L}_1v_{N-1}-\hat{L}_1w_{N-1})]^T.$

Since $(J - h^2\hat{D}U)$ is a monotone matrix, by Lemmas 6 and 7, for $-\infty < u^* \le 0$ and $0 < u^* < \pi^2/(b-a)^2$, respectively. Hence by Theorem 2, $(J - h^2\hat{D}U)$ is nonsingular. Hence,

(71) $$[v - w] = (J - h^2\hat{D}U)^{-1}(b_1 + b_2).$$

Now $\quad u_* \le u \le u^*, \qquad$ so that $\; U_* \le U \le U^*,$

where U, U_*, U^* are the matrices given in Definitions 7, 8, 9. Hence

$$(J - h^2\hat{D}U) \ge (J - h^2\hat{D}U^*).$$

If both of these matrices are monotone then by Theorem 4,

(72) $$(J - h^2\hat{D}U)^{-1} \le (J - h^2\hat{D}U^*)^{-1}.$$

Using (72) in (70),

(73) $$[v - w] \le (J - h^2\hat{D}U^*)^{-1}(b_1 + b_2).$$

According to Lemma 5, writing $\hat{\beta}_{1n} - 1 = \theta_n h^2$, $1 \le n \le N-1$, we get

$$(J - h^2\hat{D}U^*) = J - h^2(\, I + h^2\hat{\theta}\,)U^* = (J - h^2U^*) - h^4\hat{\theta}\, U^*,$$

where $\hat{\theta} = \mathrm{diag}(\theta_1, \theta_2, \ldots, \theta_{N-1})$ and by Corollary 4, $\| \hat{\theta} \| \le \Theta$. If

(74) $$\| (J - h^2U^*)^{-1}h^4\hat{\theta}U^* \| \le k < 1,$$

then by Lemma 2, the matrix $[I - (J - h^2U^*)^{-1}h^4\hat{\theta}U^*]^{-1}$ exists and

$$\| [I - (J - h^2U^*)^{-1}\, h^4\hat{\theta}U^*]^{-1}\|_\infty \le \frac{1}{1-k}.$$

So, $\quad (J - h^2\hat{D}U^*)^{-1} = [I - (J - h^2U^*)^{-1}\, h^4\hat{\theta}U^*]^{-1}\, (J - h^2U^*)^{-1}.$

Hence from (73), we get

$$[v - w] \le [I - (J - h^2U^*)^{-1}\, h^4\hat{\theta}U^*]^{-1}\, (J - h^2U^*)^{-1}\, (b_1 + b_2).$$

Hence for $1 \le i \le N-1$,

$$(75)\quad |v_i - w_i| \le \| [v - w] \|_\infty \le \| [I - (J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*]^{-1} \|_\infty$$
$$\cdot \left(\| (J - h^2U^*)^{-1} b_1 \|_\infty + \| (J - h^2U^*)^{-1} b_2 \|_\infty \right).$$

Let $J - h^2U^* = (\hat{d}_{nm})_{n,m=1}^{N-1}$, and $(J - h^2U^*)^{-1} = (d_{nm})_{n,m=1}^{N-1}$.

Now we shall analyze the situation separately for the two cases.

Case 1: $-\infty < u^* < 0$.

By Lemmas 6 and 10, $J - h^2\hat{D}U$ and $J - h^2\hat{D}U^*$ are monotone for all h, provided $\Theta h^2 \le 1$. Hence for these h, the inequality (72) holds good. Now, $J - h^2U^*$ is irreducibly diagonally dominant with nonpositive off-diagonal elements and positive diagonal elements. Hence by Corollary 2, $(J - h^2U^*)^{-1} > \underline{0}$, i.e., $d_{nm} > 0$, for $1 \le n, m \le N-1$. By Lemma 3.1 of Baboo [7],

$$(J - h^2U^*)^{-1}_{n,m} = d_{nm} = \begin{cases} \dfrac{\sinh(n\theta).\sinh(N-m)\theta}{\sinh(N\theta).\sinh\theta}; & n \le m \\[2ex] \dfrac{\sinh(m\theta).\sinh(N-n)\theta}{\sinh(N\theta).\sinh\theta}; & n \ge m \end{cases}$$

where $\sinh(\theta/2) = \frac{h}{2}\sqrt{-u^*}$.

Now we shall calculate $\| (J - h^2U^*)^{-1} \|_\infty$.

Let a_m denote the sum of the elements in the m-th row of the matrix $J - h^2U^*$. Then, for $1 \le n \le N-1$,

$$\sum_{m=1}^{N-1} d_{nm}a_m = \sum_{m=1}^{N-1} d_{nm} \sum_{l=1}^{N-1} \hat{d}_{ml} = \sum_{l=1}^{N-1}\left(\sum_{m=1}^{N-1} d_{nm}\hat{d}_{ml}\right) = \sum_{l=1}^{N-1} \delta_{nl} = 1.$$

Since, for $1 \le m \le N-1$, $a_m \ge -h^2u^*$, we have

$$-h^2u^* \sum_{m=1}^{N-1} d_{nm} \le \sum_{m=1}^{N-1} d_{nm}a_m = 1, \quad \text{for } 1 \le n \le N-1.$$

So, $$\sum_{m=1}^{N-1} d_{nm} \le \frac{1}{-h^2u^*}, \qquad \text{for } 1 \le n \le N-1.$$

Hence,

$$(76) \qquad \|(J - h^2U^*)^{-1}\|_\infty = \max_{1\le n\le N-1} \sum_{m=1}^{N-1} d_{nm} \le \frac{1}{-h^2u^*}.$$

Hence by Corollary 4,

$$\|(J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*\|_\infty \le \|(J - h^2U^*)^{-1}\|_\infty\, h^4\, \|\hat{\theta}\|_\infty\, \|U^*\|_\infty$$

$$\le \frac{1}{-h^2u^*} h^4\Theta(-u^*) = \Theta h^2 = k, \text{ say.}$$

Thus, as stated in (74), if $\Theta h^2 < 1$, then the matrix

$[I - (J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*]^{-1}$ exists and

$$(77) \qquad \|[I - (J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*]^{-1}\|_\infty \le \frac{1}{1-\Theta h^2} = C_1, \text{ say.}$$

Let $(J - h^2U^*)^{-1}b_1 = [\tilde{V}_1, \tilde{V}_2, \ldots\ldots, \tilde{V}_{N-1}]^T$,

where $\tilde{V}_i = (v_0 - w_0)d_{i1} + (v_N - w_N)d_{iN-1}, \quad 1 \le i \le N-1.$

Then $\|(J - h^2U^*)^{-1}b_1\|_\infty \le \max\left\{|v_0 - w_0|\ ,\ |v_N - w_N|\right\} \|\tilde{W}\|_\infty$,

where $\tilde{W} = [\tilde{W}_1, \tilde{W}_2, \ldots\ldots, \tilde{W}_{N-1}]^T$, with $\tilde{W}_i = d_{i1} + d_{i,N-1}$, $1 \le i \le N-1$.

So, $$\tilde{W}_i = \frac{\sinh(N-i)\theta}{\sinh(N\theta)} + \frac{\sinh(i\theta)}{\sinh(N\theta)} = \frac{\sinh(N-i)\theta + \sinh(i\theta)}{\sinh(N\theta)}$$

$$= \frac{2\sinh\frac{N\theta}{2}\,.\cosh\left(\frac{N-2i}{2}\right)\theta}{2\sinh\frac{N\theta}{2}\,.\cosh\frac{N\theta}{2}} = \frac{\cosh\left(\frac{N-2i}{2}\right)\theta}{\cosh\frac{N\theta}{2}} \le 1,$$

since, cosh is a monotonically increasing function in $[0, \infty)$. So,

$$(78) \qquad \|(J - h^2U^*)^{-1}b_1\|_\infty \le \max\left\{|v_0-w_0|\ ,\ |v_N-w_N|\right\}.$$

Again, using (76),

$$\| (J - h^2U^*)^{-1}b_2 \|_\infty \le \| (J - h^2U^*)^{-1} \|_\infty \| b_2 \|_\infty$$

$$\le \frac{1}{-h^2u^*} h^2 \max_{1\le j\le N-1} | \hat{L}_1 v_j - \hat{L}_1 w_j |.$$

Hence,

$$\| (J - h^2U^*)^{-1}b_2 \|_\infty \le \frac{1}{-u^*} \max_{1\le j\le N-1} | \hat{L}_1 v_j - \hat{L}_1 w_j |. \tag{79}$$

Using (77), (78) and (79) in (75) the result of Case 1 follows.

<u>Case 2</u>: $0 < u^* < \pi^2/(b-a)^2$.

By Lemmas 7 and 11, $J - h^2\hat{D}U$ and $J - h^2\hat{D}U^*$ are monotone matrices for all $h < H_1$, provided $\Theta h^2 \le 1$ where H_1 is the smallest positive root of the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

Hence for these h, the inequality (72)holds good. Again by Lemma 14, $J - h^2U^*$ is a monotone matrix for all $h < H_2$, where H_2 is the smallest positive root of the equation:

$$H^2u^* - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

Then by Theorem 2, $(J - h^2U^*)^{-1} \ge \underline{0}$, i.e., $d_{nm} \ge 0$. By Lemma 3.2 of Chawla [45],

$$(J - h^2U^*)^{-1}_{n,m} = d_{nm} = \begin{cases} \dfrac{\sin(n\theta).\sin(N-m)\theta}{\sin(N\theta).\sin\theta}; & n \le m \\[2ex] \dfrac{\sin(m\theta).\sin(N-n)\theta}{\sin(N\theta).\sin\theta}; & n \ge m, \end{cases}$$

where $\sin(\theta/2) = \frac{h}{2}\sqrt{u^*}$.

Now we shall calculate $\| (J - h^2U^*)^{-1} \|_\infty$.

$$\sum_{m=1}^{N-1} |d_{nm}| = \sum_{m=1}^{n} d_{nm} + \sum_{m=n+1}^{N-1} d_{nm}$$

$$= \sum_{m=1}^{n} \frac{\sin(m\theta).\sin(N-n)\theta}{\sin(N\theta).\sin\theta} + \sum_{m=n+1}^{N-1} \frac{\sin(n\theta).\sin(N-m)\theta}{\sin(N\theta).\sin\theta}$$

$$\le \sum_{m=1}^{n} \frac{m\theta.(N-n)\theta}{\sin(N\theta).\sin\theta} + \sum_{m=n+1}^{N-1} \frac{n\theta.(N-m)\theta}{\sin(N\theta).\sin\theta}$$

$$\le \frac{(N-n)\theta\,\frac{n(n+1)\theta}{2} + n\theta\frac{(N-n-1)(N-n)\theta}{2}}{\sin(N\theta).\sin\theta} \le \frac{N^2}{8}\,\frac{N\theta}{\sin(N\theta)}\,\frac{\theta}{\sin\theta}.$$

So,

(80) $$\| (J - h^2U^*)^{-1} \|_\infty \le \frac{N^2}{8}\,\frac{N\theta}{\sin(N\theta)}\,\frac{\theta}{\sin\theta}.$$

Hence, $\|(J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*\|_\infty \le h^4 \|(J - h^2U^*)^{-1}\| \|\hat{\theta}\| \|U^*\|$, so that

(81) $$\|(J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*\|_\infty \le \Theta h^2 u^* \frac{(b-a)^2}{8}\,\frac{N\theta}{\sin(N\theta)}\,\frac{\theta}{\sin\theta} = k, \text{ say.}$$

Thus as stated in (74), if $k < 1$, i.e., if

(82) $$\Theta h^2 < \frac{8}{(b-a)^2 u^*},$$

then the matrix $[I - (J - h^2U^*)^{-1} h^4\hat{\theta}U^*]^{-1}$ exists and

(83) $$\|[I - (J - h^2U^*)^{-1} h^4\hat{\theta}\, U^*]^{-1}\|_\infty \le \frac{1}{1-k} = C_2, \text{ say.}$$

As in the Case 1,

$$\|(J - h^2U^*)^{-1}b_1\|_\infty \le \max\left\{|v_0-w_0|\ ,\ |v_N-w_N|\right\} \|\ W\ \|,$$

where $\tilde{W} = [\tilde{W}_1, \tilde{W}_2, \ldots\ldots, \tilde{W}_{N-1}]^T$, with $\tilde{W}_i = d_{i1} + d_{i,N-1}$, $1 \le i \le N-1$.

So, $$\tilde{W}_i = \frac{\sin(N-i)\theta}{\sin(N\theta)} + \frac{\sin(i\theta)}{\sin(N\theta)}$$

$$= \frac{2\sin\frac{N\theta}{2}\ .\cos\left(\frac{N-2i}{2}\right)\theta}{2\sin\frac{N\theta}{2}\ .\cos\frac{N\theta}{2}} = \frac{\cos\left(\frac{N-2i}{2}\right)\theta}{\cos\frac{N\theta}{2}} \le \frac{1}{\cos\frac{N\theta}{2}},\quad 1 \le i \le N-1,$$

so that,

$$(84)\qquad \| (J - h^2U^*)^{-1}b_1 \|_\infty \le \frac{1}{\cos\frac{N\theta}{2}} \max\left\{|v_0-w_0|\ ,\ |v_N-w_N|\right\}.$$

Again, by (80),

$$\| (J - h^2U^*)^{-1}b_2 \|_\infty \le \| (J - h^2PU^*)^{-1} \|_\infty \| b_2 \|_\infty$$

$$\le \frac{N^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} h^2 \max_{1\le j\le N-1} |\hat{L}_1 v_j - \hat{L}_1 w_j|,$$

or,

$$(85)\qquad \| (J - h^2U^*)^{-1}b_2 \|_\infty \le \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} \max_{1\le j\le N-1} |\hat{L}_2 v_j - \hat{L}_2 w_j|.$$

Using (81)-(85) in (75) the result of Case 2 follows.

Stability of Stormer's usual method (9) is discussed in Keller [115], in case when $-\infty < u^* < 0$, [Theorem 3.2.1, Keller]. Using the analysis in the proof of Theorem 10, it is possible to give an alternate proof for the stability of Stormer's method both for the cases $-\infty < u^* < 0$ and $0 < u^* < \pi^2/(b-a)^2$ as follows:

<u>Proposition 1:</u> Let L_1 be the linear difference operator associated with Stormer's method (9). Then

$$L_1 v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} - f(x_i, v_i) = 0;\quad 1 \le i \le N-1,$$

If $f(x,y)$ has continuous derivatives with respect to y, satisfying

$$u_* \le \frac{\partial f}{\partial y} \le u^*,$$

then L_1 is stable in the sense that for all net functions $\{v_i\},\{w_i\}$

$$|v_i - w_i| \le M \left\{ \max\left(|v_0 - w_0|, |v_N - w_N|\right) + \max_{1 \le j \le N-1} |L_1 v_j - L_1 w_j| \right\},$$

for $1 \le i \le N-1$, for some constant M and some suitable restriction on h given in the following two cases:

<u>Case1 :</u> $\quad -\infty < u^* < 0.$

Then L_1 is stable for all h with $M = M_1$, where

$$M_1 = \max\left\{1 \; , \; \frac{1}{-u^*}\right\}.$$

<u>Case 2:</u> $\quad 0 < u^* < \pi^2/(b-a)^2.$

Then L_1 is stable for all $h < H_0$, where H_0 is the smallest positive root of the equation:

$$H^2 u^* - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

with $M = M_2$, where $M_2 = \max\left\{\frac{1}{\cos\frac{N\theta}{2}} \; , \; \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta}\right\}.$

<u>Proof:</u> If $\{v_i\}$ and $\{w_i\}$ are any two net functions, then as in Theorem 10,

$$h^2[L_1 v_i - L_1 w_i] = -(v_{i-1} - w_{i-1}) + (2 - h^2 u_i)(v_i - w_i) - (v_{i+1} - w_{i+1}),$$

where $\quad u_i = \frac{\partial}{\partial y} f(x_i, w_i + \xi_i(v_i - w_i)), \quad 1 \le i \le N-1.$

In matrix notation , the above system of equations becomes,

(86) $$(J - h^2 U)\,[v-w] = b_1 + b_2,$$

where J, U are $(N-1)\times(N-1)$ matrices given by Definitions 4, 7,

$$[v - w] = [(v_1 - w_1), (v_2 - w_2), \ldots\ldots, (v_{N-1} - w_{N-1})]^T,$$

$$b_1 = [(v_0 - w_0), 0, \ldots\ldots\ldots\ldots, 0, (v_N - w_N)]^T,$$

$$b_2 = h^2[(L_1v_1 - L_1w_1),(L_1v_2-L_1w_2),\ldots\ldots,(L_1v_{N-1}-L_1w_{N-1})]^T.$$

Since $U \le U^*$, $(J - h^2U) \ge (J - h^2U^*)$.

If both of these matrices are monotone, then by Theorem 4,

$$(87) \qquad (J - h^2U)^{-1} \le (J - h^2U^*)^{-1}.$$

Using (87) in (86), we get

$$[v - w] \le (J - h^2U^*)^{-1}(b_1 + b_2).$$

Hence for $1\le i\le N-1$,

$$(88) \quad |v_i - w_i| \le \|[v - w]\|_\infty \le \|(J - h^2U^*)^{-1}b_1\|_\infty+\|(J - h^2U^*)^{-1}b_2\|_\infty.$$

<u>Case 1:</u> $-\infty < u^* < 0.$

Now, $J - h^2U$ and $J - h^2U^*$ are irreducibly diagonally dominant with non-positive off-diagonal elements and positive diagonal elements. Hence by corollary 2, they are monotone matrices. Hence, the inequality (87) holds good. Similar to (79), in this situation

$$(89) \qquad \|(J - h^2U^*)^{-1}b_2\|_\infty \le \frac{1}{-u^*} \max_{1\le j\le N-1} |L_1v_j - L_1w_j|,$$

and $\|(J - h^2U^*)^{-1}b_1\|_\infty$ is as given in (78). Using (78) and (89) in (88) the result of Case 1 follows.

<u>Case 2:</u> $0 < u^* < \pi^2/(b-a)^2.$

By Lemma 14, $J - h^2U$ and $J - h^2U^*$ are monotone matrices for all $h < H_0$, where H_0 is the smallest positive root of the equation

$$H^2u^* - 4\sin^2\frac{\pi H}{2(b-a)} = 0.$$

Hence, the inequality (87) holds good. Similar to (85), we get

(90) $$\| (J - h^2U^*)^{-1}b_2 \|_\infty \le \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)\sin\theta} \max_{1\le j\le N-1} |L_2v_j - L_2w_j|,$$

and $\| (J - h^2U^*)^{-1}b_1 \|_\infty$ is as given in (84). Using (84) and (90) in (88), the result of Case 2 follows.

Now as an application of the stability theory of the optimal method we shall establish a relation between the discretization error and the local truncation error for this method.

Let $\mathcal{L}_h$ be a finite difference operator to solve a BVP (1) of the form

(I) $$\mathcal{L}\, y(x) \equiv -y'' - f(x,y) = 0, \qquad a < x < b,$$

$$y(a) = A, \quad y(b) = B,$$

where f(x,y) satisfies the conditions stated in (1).

According to Keller [115], let us define the following.

<u>Definition 15:</u> The local truncation errors, in $\mathcal{L}_h$, as an approximation to $\mathcal{L}$, for any smooth function $\omega(x)$, is defined by

$$\tau_j[\omega] \equiv \mathcal{L}_h\, \omega(x_j) - \mathcal{L}\, \omega(x_j), \quad 1 \le j \le N-1.$$

<u>Corollary 7:</u> Let f(x,y) have continuous derivative with respect to y satisfying $u_* \le \frac{\partial f}{\partial y} \le u^*$. Then the numerical solution $\{y_j\}$ of the difference equation

$$\hat{L}_i v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} - \hat{\beta}_{i,i} f(x_i, v_i) = 0; \qquad 1 \le i \le N-1,$$

and the solution y(x) of the BVP (I) satisfy the relation

$$| y_j - y(x_j) | \le M \max_{1\le j\le N-1} |\hat{\tau}_j^1[y]|, \qquad 0 \le j \le N,$$

where $\quad \hat{\tau}_j^1[\omega] \equiv \hat{L}_1\omega(x_j) - \mathcal{L}\,\omega(x_j), \qquad 1 \le j \le N-1,$

and M is a constant described in the following two Cases.

<u>Case 1</u> : $\qquad -\infty < u^* < 0.$

$M = \hat{M}_1 = \dfrac{1}{1-\Theta h^2} \max\left\{1\ ,\ \dfrac{1}{-u^*}\right\}$, for all h satisfying $\Theta h^2 < 1$.

<u>Case 2</u> : $\qquad 0 < u^* < \pi^2/(b-a)^2.$

$$M = \hat{M}_2 = \frac{1}{1-\ \Theta h^2 u^* \dfrac{(b-a)^2}{8} \dfrac{N\theta}{\sin(N\theta)} \dfrac{\theta}{\sin\theta}}$$

$$.\max\left\{\frac{1}{\cos\frac{N\theta}{2}}\ ,\ \frac{(b-a)^2}{8}\ \frac{N\theta}{\sin(N\theta)}\ \frac{\theta}{\sin\theta}\right\},$$

for all $h < \min\{H_1,H_2\}$, H_1 is the smallest positive root of the equation:

$$H^2u^*(1 + \Theta H^2) - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

and H_2 is the smallest positive root of the equation:

$$H^2u^* - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

provided $\Theta h^2 < \min\left\{1\ ,\ \dfrac{8}{(b-a)^2u^*}\right\}$.

<u>Proof:</u> From (I) and the definition of $\hat{L}_1$, evaluated at $x = x_j$, we have by the linearity of $\hat{L}_1$ and the Definition 15,

$$\hat{L}_1[y_j - y(x_j)] = \hat{L}_1 y_j - \hat{L}_1 y(x_j) = 0 - \hat{L}_1 y(x_j)$$

$$= \mathcal{L}\ y(x_j) - \hat{L}_1 y(x_j) = -\hat{\tau}_j^1[y].$$

Now since, $\quad y_0 - y(x_0) = y_N - y(x_N) = 0,$

applying Theorem 10, with $v_j - w_j = y_j - y(x_j)$, the result follows.

<u>Theorem 11:</u> Let $\hat{L}_2$ be the linear difference operator associated with the optimal method corresponding to the usual Cowell's method and a net function $\{v_i\}$ be defined as

$$\hat{L}_2 v_i \equiv - \frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} -$$

$$\left\{ \hat{\beta}_{0,i} f(x_{i-1}, v_{i-1}) + \hat{\beta}_{1,i} f(x_i, v_i) + \hat{\beta}_{2,i} f(x_{i+1}, v_{i+1}) \right\},$$

where $\hat{\beta}_{k,i}$; $k = 0,1,2$; $1 \le i \le N-1$, are the optimal coefficients corresponding to the usual coefficients $\beta_0 = \frac{1}{12}$, $\beta_1 = \frac{10}{12}$, $\beta_2 = \frac{1}{12}$ and Φ be as before, so that $|\hat{\beta}_{k,i} - \beta_k| \le \Phi h^2$, $k = 0,1,2$; $1 \le i \le N-1$. Assume that $f(x,y)$ has continuous derivatives with respective to y, satisfying

$$u_* \le \frac{\partial f}{\partial y} \le u^*.$$

Then $\hat{L}_2$ is stable in the sense that for all net functions $\{v_i\}, \{w_i\}$

$$|v_i - w_i| \le M \left\{ \max\left(|v_0 - w_0|, |v_N - w_N| \right) + \max_{1 \le j \le N-1} |\hat{L}_2 v_j - \hat{L}_2 w_j| \right\},$$

$1 \le i \le N-1$, for some constant M and some suitable restriction on h given in the following two cases.

<u>Case 1 :</u> $-\infty < u^* < 0$.

Then $\hat{L}_2$ is stable with $M = \hat{M}_3$ where

$$\hat{M}_3 = \frac{1}{1-\Phi h^2} \max \left\{ \left(1 + \frac{h^2 u^*}{1 + \frac{h^2 u^*}{12}} \right), \frac{1}{-u^*} \right\}, \quad \text{for all } h < \min\,(H_3, H_4),$$

where $H_3 \le \min \left\{ \sqrt{\frac{6}{-u_*}}, \sqrt{\frac{6}{-u^*}} \right\}$, and $H_4 \le \sqrt{\frac{12}{-u^*}}$, provided $\Phi h^2 \le \frac{1}{12}$.

<u>Case 2:</u> $0 < u^* < \pi^2/(b-a)^2$.

Then $\hat{L}_2$ is stable with $M = \hat{M}_4$ where

$$\hat{M}_4 = \frac{1}{1-\dfrac{\Phi h^2 u^*}{1+\dfrac{h^2u^*}{12}}\dfrac{(b-a)^2}{8}\dfrac{N\theta}{\sin(N\theta)}\dfrac{\theta}{\sin\theta}}\,\cdot$$

$$\max\left\{\left(1+\frac{8h^2}{(b-a)^2}\right)\frac{1}{\cos\frac{N\theta}{2}},\ \frac{1}{1+\dfrac{h^2u^*}{12}}\frac{(b-a)^2}{8}\frac{N\theta}{\sin(N\theta)}\frac{\theta}{\sin\theta}\right\},$$

for all $h < \min\{H_5, H_6\}$,

provided $\Phi h^2 \le \frac{1}{12}$, where $H_5 \le \min\{h_1, h_2\}$, with $h_1 = \sqrt{\frac{6}{-u_*}}$, h_2 and H_6 are the smallest positive roots of the respective equation:

$$H^2u^*\left[(1+3\Phi H^2) - (\tfrac{1}{12}+\Phi H^2)4\sin^2\frac{\pi H}{2(b-a)}\right] - 4\sin^2\frac{\pi H}{2(b-a)} = 0,$$

and

$$h^2u^*\left(\frac{1}{4\sin^2\frac{\pi h}{2(b-a)}} - \frac{1}{12}\right) = 1.$$

<u>Proof:</u> If $\{v_i\}$ and $\{w_i\}$ are any two net functions, then

$$h^2\hat{L}_2v_i = -(v_{i-1} - 2v_i + v_{i+1}) - h^2\sum_{k=0}^{2}\hat{\beta}_{k,i}f(x_{i+k-1}, v_{i+k-1}),$$

$$h^2\hat{L}_2w_i = -(w_{i-1} - 2w_i + w_{i+1}) - h^2\sum_{k=0}^{2}\hat{\beta}_{k,i}f(x_{i+k-1}, w_{i+k-1}).$$

So, $h^2[\hat{L}_2v_i - \hat{L}_2w_i] = -(v_{i-1} - w_{i-1}) + 2(v_i - w_i) - (v_{i+1} - w_{i+1})$

$$-h^2\sum_{k=0}^{2}\hat{\beta}_{k,i}(v_{i+k-1}-w_{i+k-1})\frac{\partial}{\partial y}f(x_{i+k-1}, w_{i+k-1}+\xi_{i+k-1}(v_{i+k-1}-w_{i+k-1})).$$

Let

$u_{i+k-1} = \frac{\partial}{\partial y}f(x_{i+k-1}, w_{i+k-1}+\xi_{i+k-1}(v_{i+k-1}-w_{i+k-1}))$, $k=0,1,2;\ 1\le i\le N-1$.

Then the above equation becomes

$$h^2[\hat{L}_2v_i - \hat{L}_2w_i] = (-1-h^2\hat{\beta}_{0,i}u_{i-1})(v_{i-1}-w_{i-1}) + (2-h^2\hat{\beta}_{1,i}u_i)(v_i-w_i)$$

$$+ (-1-h^2\hat{\beta}_{2,i}u_{i+1})(v_{i+1}-w_{i+1}), \quad \text{for } 1 \le i \le N-1.$$

In matrix notation, this system of equations reads

$$(J - h^2\hat{P}U)\ [v - w] = b_1 + b_2,$$

where J, $\hat{P}$, U are $(N-1)\times(N-1)$ matrices given by Definitions 4, 6,7,

$$[v-w] = [(v_1-w_1),(v_2-w_2),\ldots\ldots,(v_{N-1}-w_{N-1})]^T,$$

$$b_1 = [(1+h^2\hat{\beta}_{0,1}u_0)(v_0-w_0),0,\ldots\ldots,0,(1+h^2\hat{\beta}_{2,N-1}u_N)(v_N-w_N)]^T,$$

$$b_2 = h^2[(\hat{L}_2v_1-\hat{L}_2w_1),(\hat{L}_2v_2-\hat{L}_2w_2),\ldots\ldots,(\hat{L}_2v_{N-1}-\hat{L}_2w_{N-1})]^T.$$

If $(J - h^2\hat{P}U)$ is a monotone matrix, then it is nonsingular, by Theorem 2. So,

$$\text{(91)} \qquad [v - w] = (J - h^2\hat{P}U)^{-1}(b_1 + b_2).$$

Now $u_* \le u \le u^*$, so that $U_* \le U \le U^*$,

where U, U_*, U^* are the matrices given by Definitions 7, 8, 9.

Hence, $$(J - h^2\hat{P}U) \ge (J - h^2\hat{P}U^*).$$

If both of these matrices are monotone, then by Theorem 4,

$$\text{(92)} \qquad (J - h^2\hat{P}U)^{-1} \le (J - h^2\hat{P}U^*)^{-1}.$$

Using (92) in (91), we get

$$\text{(93)} \qquad [v - w] \le (J - h^2\hat{P}U^*)^{-1}(b_1 + b_2).$$

According to Lemma 4, we can write,

$$\hat{\beta}_{in} - \beta_i = \phi_{in}h^2, \quad i = 0,1,2; \quad 1 \le n \le N-1.$$

Let $\hat{\phi} = (\hat{\phi}_{ij})_{i,j=1}^{N-1}$ be a tridiagonal matrix, where

$\hat{\phi}_{ii} = \phi_{1,i}$, $1 \le i \le N-1$; $\hat{\phi}_{i,i-1} = \phi_{0,i}$, $2 \le i \le N-1$; $\hat{\phi}_{i,i+1} = \phi_{2,i}$, $1 \le i \le N-2$.

Then,

$$(J - h^2\hat{P}U^*) = J - h^2(P + h^2\hat{\phi})U^* = (J - h^2PU^*) - h^4\hat{\phi}U^*,$$

where P is a matrix given by Definition 10. If

$$\| (J - h^2PU^*)^{-1} h^4\hat{\phi}U^* \|_\infty \le k < 1, \tag{94}$$

then by Lemma 2, $[I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}$ exists and

$$\| [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1} \|_\infty \le \frac{1}{1-k}.$$

So, $\quad (J - h^2\hat{P}U^*)^{-1} = [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}(J - h^2PU^*)^{-1}.$

Hence from (93) we get,

$$[v - w] \le [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}(J - h^2PU^*)^{-1}(b_1 + b_2),$$

and for $1 \le i \le N-1$,

$$|v_i - w_i| \le \| [v - w] \|_\infty \le \| [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1} \|_\infty \cdot \tag{95}$$

$$\cdot \Big(\| (J-h^2PU^*)^{-1}b_1 \|_\infty + \| (J-h^2PU^*)^{-1}b_2 \|_\infty \Big).$$

Let $J - h^2PU^* = (\hat{g}_{nm})_{n,m=1}^{N-1}$, and $(J - h^2PU^*)^{-1} = (g_{nm})_{n,m=1}^{N-1}$.

<u>Case 1:</u> $\quad -\infty < u^* < 0$.

By Lemma 8 and Lemma 12, $J - h^2\hat{P}U$ and $J - h^2\hat{P}U^*$ are monotone matrices for all $h < H_3$, provided $\Phi h^2 \le \frac{1}{12}$,

where $$H_3 \le \min\left\{\sqrt{\frac{6}{-u_*}}\,,\ \sqrt{\frac{6}{-u^*}}\right\}.$$

Hence for these h, the relations (91) and (92) hold good. Again by Lemma 16, $J - h^2PU^*$ is monotone for all $h < H_4$,

where $$H_4 = \sqrt{\frac{12}{-u^*}}.$$

Then by Theorem 2, $(J - h^2PU^*)^{-1} \geq \underline{0}$ i.e., $g_{nm} \geq 0$. By Lemma 18, we have

$$(J - h^2 P U^*)^{-1}_{n,m} = g_{nm} = \begin{cases} \dfrac{1}{1+\dfrac{h^2u^*}{12}} \dfrac{\sinh(n\theta).\sinh(N-m)\theta}{\sinh(N\theta).\sinh\theta}; & n \leq m \\[2ex] \dfrac{1}{1+\dfrac{h^2u^*}{12}} \dfrac{\sinh(m\theta).\sinh(N-n)\theta}{\sinh(N\theta).\sinh\theta}; & n \geq m, \end{cases}$$

where $\sinh(\theta/2) = \dfrac{h}{2}\sqrt{\dfrac{-u^*}{1+\dfrac{h^2u^*}{12}}}$.

Now we shall calculate $\|(J - h^2PU^*)^{-1}\|_\infty$. Let a_m denote the sum of the elements in the m-th row of the matrix $J - h^2PU^*$. Then as in the Case 1 of Theorem 10,

$$\sum_{m=1}^{N-1} g_{nm}a_m = 1; \qquad \text{for } 1 \leq n \leq N-1.$$

Now, $a_1 = a_{N-1} = 1 - \frac{11}{12} h^2u^* \geq - h^2u^*$, if $h \leq \sqrt{\frac{12}{-u^*}}$.

Also, $a_m = - h^2u^*$, for $2 \leq m \leq N-2$.

So, $a_m \geq - h^2u^*$, for $1 \leq m \leq N-1$, if $h \leq \sqrt{\frac{12}{-u^*}}$.

So, $$- h^2u^* \sum_{m=1}^{N-1} g_{nm} \leq \sum_{m=1}^{N-1} g_{nm}a_m = 1, \quad \text{for } 1 \leq n \leq N-1,$$

and $$\sum_{m=1}^{N-1} g_{nm} \leq \frac{1}{- h^2u^*}, \qquad \text{for } 1 \leq n \leq N-1.$$

So, $$\| (J - h^2PU^*)^{-1}\|_\infty = \max_{1 \le n \le N-1} \sum_{m=1}^{N-1} g_{nm} \le \frac{1}{-h^2u^*}.$$

Hence, using Corollary 3, we have

$$\|(J - h^2PU^*)^{-1} h^4\hat{\phi}\, U^*\|_\infty \le \|(J - h^2PU^*)^{-1}\|_\infty\, h^4 \,\|\hat{\phi}\|_\infty \,\| U^* \|_\infty$$

$$\le \frac{1}{-h^2u^*} h^4\Phi\, (-u^*) = \Phi h^2.$$

Thus as stated in (94), if $\Phi h^2 < 1$, then the matrix

$$[I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1} \text{ exists and}$$

(96) $$\| [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}\|_\infty \le \frac{1}{1-\Phi h^2} = C_3, \text{ say.}$$

Let $(J - h^2PU^*)^{-1}b_1 = [\tilde{V}_1, \tilde{V}_2, \ldots\ldots\ldots\ldots, \tilde{V}_{N-1}]^T$ where

$$\tilde{V}_i = (1+h^2\hat{\beta}_{0,1}u_0)(v_0-w_0)g_{i1} + (1+h^2\hat{\beta}_{2,N-1}u_N)(v_N-w_N)g_{iN-1}, \quad 1\le i\le N-1,$$

and $\tilde{W} = [\tilde{W}_1, \tilde{W}_2, \ldots\ldots\ldots\ldots, \tilde{W}_{N-1}]^T$,

with $\tilde{W}_i = g_{i1} + g_{i,N-1}$, $\quad 1 \le i \le N-1$.

Then

$$\|(J-h^2PU^*)^{-1}b_1\|_\infty \le \left\{1+h^2(\tfrac{1}{12} + \Phi h^2)u^*\right\}.\max\left\{|v_0-w_0| \;,\; |v_N-w_N|\right\}\| \tilde{W} \|_\infty.$$

Now as in the Case 1 of Theorem 10, for $1 \le i \le N-1$

$$\tilde{W}_i = g_{i1} + g_{i,N-1} = \frac{1}{1+\frac{h^2u^*}{12}}\left(\frac{\sinh(N-i)\theta}{\sinh(N\theta)} + \frac{\sinh(i\theta)}{\sinh(N\theta)}\right) \le \frac{1}{1+\frac{h^2u^*}{12}}$$

So, $\| \tilde{W} \|_\infty \le \dfrac{1}{1+\frac{h^2u^*}{12}}$. Using $\Phi h^2 < 1$,

(97) $$\|(J-h^2PU^*)^{-1}b_1\|_\infty \le \frac{\left\{1+h^2(\frac{1}{12} + \Phi h^2)u^*\right\}}{1+\frac{h^2u^*}{12}}.\max\left\{|v_0-w_0| \;,\; |v_N-w_N|\right\}$$

$$< \left(1 + \frac{h^2u^*}{1+\frac{h^2u^*}{12}}\right).\max \left\{|v_0-w_0| \ , \ |v_N-w_N|\right\}.$$

Again, $\| (J - h^2PU^*)^{-1}b_2 \|_\infty \le \| (J - h^2PU^*)^{-1} \|_\infty \| b_2 \|_\infty$

$$\le \frac{1}{-h^2u^*} h^2 \max_{1\le j\le N-1} | \hat{L}_2v_j - \hat{L}_2w_j|.$$

So,

$$(98) \qquad \|(J - h^2PU^*)^{-1}b_2\|_\infty \le \frac{1}{-u^*} \max_{1\le j\le N-1} | \hat{L}_2v_j - \hat{L}_2w_j|.$$

Using (96), (97) and (98) in (95) the result of Case 1 follows.

<u>Case 2</u>: $0 < u^* < \pi^2/(b-a)^2$.

By Lemma 9 and Lemma 13, $J - h^2\hat{P}U$ and $J - h^2\hat{P}U^*$ are monotone for all $h < H_5$, provided $\Phi h^2 \le \frac{1}{12}$, where $H_5 \le \min\{h_1,h_2\}$, with $h_1 = \sqrt{\frac{6}{-u_*}}$ and h_2 is the smallest positive root of the equation :

$$H^2u^*\left[(1 + 3\Phi H^2) - (\frac{1}{12} + \Phi H^2)4\sin^2 \frac{\pi H}{2(b-a)}\right] - 4\sin^2 \frac{\pi H}{2(b-a)} = 0.$$

Hence for these h, the relations (91) and (92) hold good. Again by Lemma 17, $J - h^2PU^*$ is monotone for all $h < H_6$, where H_6 is the root of the equation,

$$h^2u^* \left(\frac{1}{4\sin^2 \frac{\pi h}{2(b-a)}} - \frac{1}{12}\right) = 1.$$

So, by Theorem 2, $(J - h^2PU^*)^{-1} \ge \underline{0}$, i.e., $g_{nm} \ge 0$.

By Lemma 19, we get

$$(J - h^2 P U^*)^{-1}_{n,m} = g_{nm} = \begin{cases} \dfrac{1}{1+\dfrac{h^2u^*}{12}} \dfrac{\sin(n\theta).\sin(N-m)\theta}{\sin(N\theta).\sin\theta}; & n \le m \\ \dfrac{1}{1+\dfrac{h^2u^*}{12}} \dfrac{\sin(m\theta).\sin(N-n)\theta}{\sin(N\theta).\sin\theta}; & n \ge m, \end{cases}$$

where $\sin(\theta/2) = \dfrac{h}{2}\sqrt{\dfrac{u^*}{1 + \dfrac{h^2u^*}{12}}}$.

Now we shall calculate $\|(J - h^2PU^*)^{-1}\|_\infty$. As in the Case 2 of Theorem 10, we have

$$\sum_{m=1}^{N-1} |g_{nm}| = \sum_{m=1}^{n} g_{nm} + \sum_{m=n+1}^{N-1} g_{nm}$$

$$= \frac{1}{1+\dfrac{h^2u^*}{12}} \left[\sum_{m=1}^{n} \frac{\sin(m\theta).\sin(N-n)\theta}{\sin(N\theta).\sin\theta} + \sum_{m=n+1}^{N-1} \frac{\sin(n\theta).\sin(N-m)\theta}{\sin(N\theta).\sin\theta}\right]$$

$$\le \frac{1}{1+\dfrac{h^2u^*}{12}} \frac{N^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta},$$

and

$$\|(J - h^2PU^*)^{-1}\|_\infty \le \frac{1}{1+\dfrac{h^2u^*}{12}} \frac{N^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta}. \tag{99}$$

Hence, $\|(J - h^2PU^*)^{-1} h^4\hat{\phi}U^*\|_\infty \le \|(J - h^2PU^*)^{-1}\|_\infty h^4 \|\hat{\phi}\|_\infty \|U^*\|_\infty$,

so that

$$\|(J - h^2PU^*)^{-1}h^4\hat{\phi}U^*\|_\infty \le \frac{\Phi h^2u^*}{1+\dfrac{h^2u^*}{12}} \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} = k, \text{ say.} \tag{100}$$

Hence as stated in (94), if $k < 1$, i.e., if

$$\Phi h^2u^* < \left(1 + \frac{h^2u^*}{12}\right) \frac{8}{(b-a)^2}, \tag{101}$$

then the matrix $[I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}$ exists and

$$(102) \qquad \| [I - (J - h^2PU^*)^{-1} h^4\hat{\phi}U^*]^{-1}\|_\infty \le \frac{1}{1-k} = C_4, \text{ say.}$$

As in the Case 1,

$$\|(J-h^2PU^*)^{-1}b_1\|_\infty \le \left\{1+h^2(\tfrac{1}{12} + \Phi h^2)u^*\right\}.\max\left\{|v_0-w_0|,\ |v_N-w_N|\right\} \|\tilde{W}\|,$$

where $\tilde{W} = [\tilde{W}_1, \tilde{W}_2, \ldots\ldots, \tilde{W}_{N-1}]^T$, with

$$\tilde{W}_i = g_{i1} + g_{i,N-1},$$

$$= \frac{1}{1+\frac{h^2u^*}{12}}\left(\frac{\sin(N-i)\theta}{\sin(N\theta)} + \frac{\sin(i\theta)}{\sin(N\theta)}\right) \le \frac{1}{1+\frac{h^2u^*}{12}} \frac{1}{\cos\frac{N\theta}{2}}, \quad 1\le i\le N-1.$$

As in the Case2 of Theorem 10, using (101),

$$(103)\ \|(J-h^2PU^*)^{-1}b_1\|_\infty \le \frac{\left\{1+h^2(\frac{1}{12} + \Phi h^2)u^*\right\}}{1+\frac{h^2u^*}{12}} \frac{1}{\cos\frac{N\theta}{2}} \max\left\{|v_0-w_0|, |v_N-w_N|\right\}$$

$$\le \left(1 + \frac{8h^2}{(b-a)^2}\right) \frac{1}{\cos\frac{N\theta}{2}} \max\left\{|v_0-w_0|\ ,\ |v_N-w_N|\right\}.$$

Again, by (99),

$$\| (J - h^2PU^*)^{-1}b_2 \|_\infty \le \| (J - h^2PU^*)^{-1} \|_\infty \| b_2 \|_\infty$$

$$\le \frac{1}{1+\frac{h^2u^*}{12}} \frac{N^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} h^2 \max_{1\le j\le N-1} | \hat{L}_2v_j - \hat{L}_2w_j |,$$

so that

$$(104) \quad \|(J-h^2PU^*)^{-1}b_2\|_\infty \le \frac{1}{1+\frac{h^2u^*}{12}} \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} \max_{1\le j\le N-1} |\hat{L}_2v_j-\hat{L}_2w_j|.$$

Using (100)-(104) in (95) the result of Case 2 follows.

Now we shall prove the stability of Cowell's usual method (5) with function evaluation at three points, along the lines of the proof of Theorem 11.

Proposition 2: Let L_2 be the linear difference operator associated with Cowell's method. With the net function $\{v_i\}$ defined as

$$L_2 v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2}$$

$$\left\{\frac{1}{12} f(x_{i-1}, v_{i-1}) + \frac{10}{12} f(x_i, v_i) + \frac{1}{12} f(x_{i+1}, v_{i+1})\right\},$$

assume that $f(x,y)$ has continuous derivatives with respective to y, satisfying $$u_* \le \frac{\partial f}{\partial y} \le u^*.$$

Then L_2 is stable in the sense that for all net functions $\{v_i\},\{w_i\}$

$$|v_i - w_i| \le M \left\{\max\left(|v_0 - w_0|, |v_N - w_N|\right) + \max_{1 \le j \le N-1} |L_2 v_j - L_2 w_j|\right\},$$

$1 \le i \le N-1$, for some constant M and some suitable restriction on h given in the following two cases.

Case1 : $-\infty < u^* < 0$.

Then L_2 is stable for all $h < H_4$, with $M = M_3 = \max\left\{1, \frac{1}{-u^*}\right\}$,

for all $h < H_4$, where $H_4 \le \sqrt{\frac{12}{-u_*}}$.

Case 2: $0 < u^* < \pi^2/(b-a)^2$.

Then L_2 is stable for all $h < \min\{H_6, H_7\}$,
where $H_7 = \sqrt{\frac{12}{-\bar{u}_*}}$, $\bar{u}_* = \min(0, u_*)$, and H_6 is the smallest positive root of the equations:

$$h^2u^* \left(\frac{1}{4\sin^2 \frac{\pi h}{2(b-a)}} - \frac{1}{12} \right) = 1,$$

with $M = M_4$, where

$$M_4 = \max \left\{ \frac{1}{\cos\frac{N\theta}{2}} , \frac{1}{1+\frac{h^2u^*}{12}} \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} \right\}.$$

Proof: If $\{v_i\}$ and $\{w_i\}$ are any two net functions, then setting

$\beta_0 = \frac{1}{12}$, $\beta_1 = \frac{10}{12}$, $\beta_2 = \frac{1}{12}$ and

$u_{i+k-1} = \frac{\partial}{\partial y} f(x_{i+k-1}, w_{i+k-1} + \xi_{i+k-1}(v_{i+k-1} - w_{i+k-1}))$, $k=0,1,2;\ 1 \le i \le N-1$,

as in Theorem 11, we get

$$h^2[L_2v_i - L_2w_i] = (-1 - \frac{h^2}{12} u_{i-1})(v_{i-1}-w_{i-1}) + (2 - \frac{10}{12} h^2u_i)(v_i-w_i)$$
$$+ (-1 - \frac{h^2}{12} u_{i+1})(v_{i+1}-w_{i+1}), \quad 1 \le i \le N-1.$$

In matrix notation, this system of equations reads

$$(J - h^2PU)\ [v-w] = b_1 + b_2,$$

where J, P, U are $(N-1)\times(N-1)$ matrices given by Definitions 4,10,7;

$$[v-w] = [(v_1-w_1),(v_2-w_2),\ldots\ldots\ldots,(v_{N-1}-w_{N-1})]^T,$$

$$b_1 = [(1+\frac{h^2}{12} u_0)(v_0-w_0),0,\ldots\ldots\ldots,0,(1+\frac{h^2}{12} u_N)(v_N-w_N)]^T \quad \text{and}$$

$$b_2 = h^2[(L_2v_1-L_2w_1),(L_2v_2-L_2w_2),\ldots\ldots\ldots,(L_2v_{N-1}-L_2w_{N-1})]^T.$$

If $(J - h^2PU)$ is a nonsingular matrix, then

$$[v - w] = (J - h^2PU)^{-1}(b_1 + b_2). \tag{105}$$

Since $U \le U^*$, $\qquad (J - h^2PU) \ge (J - h^2PU^*)$.

If both of these matrices are monotone then by Theorem 4,

(106) $$(J - h^2PU)^{-1} \le (J - h^2PU^*)^{-1}.$$

Using (106) in (105) and taking norm, we get

(107) $$|v_i - w_i| \le \| [v - w] \|_\infty \le \| (J-h^2PU^*)^{-1} b_1 \|_\infty + \| (J-h^2PU^*)^{-1} b_2 \|_\infty, \quad 1 \le i \le N-1.$$

<u>Case1 :</u> $-\infty < u^* < 0.$

By Lemmas 15 and 16, $J-h^2PU$ and $J-h^2PU^*$ are monotone for all $h < H_4$, where $H_4 \le \min\left\{\sqrt{\frac{12}{-u_*}}, \sqrt{\frac{12}{-u^*}}\right\} = \sqrt{\frac{12}{-u_*}}$. Hence for all $h < H_4$, the relations (105) and (106) hold good. As in Case 1 of Theorem 11,

$$\| (J - h^2PU^*)^{-1} b_1 \|_\infty \le (1 + \frac{h^2u^*}{12}).\max\left\{|v_0 - w_0| \ , \ |v_N - w_N|\right\} \| \tilde{W} \|_\infty,$$

where $\tilde{W}$ is as defined in the prrof of Case 1 of Theorem 11, with

$$\| \tilde{W} \|_\infty \le \frac{1}{(1+ \frac{h^2u^*}{12})},$$

(108) $$\| (J - h^2PU^*)^{-1} b_1 \|_\infty \le \max\left\{|v_0 - w_0| \ , \ |v_N - w_N|\right\}.$$

Similar to (98), we get

(109) $$\| (J - h^2PU^*)^{-1} b_2 \|_\infty \le \frac{1}{-u^*} \max_{1 \le j \le N-1} |L_2 v_j - L_2 w_j|.$$

Using (108) and (109) in (107) the result of Case 1 follows.

<u>Case 2:</u> $0 < u^* < \pi^2/(b-a)^2.$

Following the proof of Lemma 9 (essesntially replacing Φ by 0), we easily obtain that $J - h^2PU$ is monotone for all $h < \min\ (H_6, H_7)$, where H_7 where $H_7 = \sqrt{\frac{12}{-\bar{u}_*}}$, $\bar{u}_*$ is smallest of 0 and u_*, and H_6 is the smallest positive root of the equation :

$$h^2u^*\left(\frac{1}{4\sin^2\frac{\pi h}{2(b-a)}} - \frac{1}{12}\right) = 1.$$

By Lemma 17, $J - h^2PU^*$ is monotone for all $h < H_6$, Hence for all $h < \min\{H_6, H_7\}$, the relations (105) and (106) hold good. As in Case 2 of Theorem 11, we get

(110) $$\|(J - h^2PU^*)^{-1}b_1\|_\infty \le \frac{1}{\cos\frac{N\theta}{2}} \max\left\{|v_0-w_0|, |v_N-w_N|\right\}.$$

Similar to (104),

(111) $$\|(J-h^2PU^*)^{-1}b_2\|_\infty \le \frac{1}{1+\frac{h^2u^*}{12}} \frac{(b-a)^2}{8} \frac{N\theta}{\sin(N\theta)} \frac{\theta}{\sin\theta} \max_{1\le j\le N-1} |L_2v_j - L_2w_j|.$$

Using (110) and (111) in (107) the result of Case 2 follows.

Now similar to Corollary 7, we shall establish the relation between the discretisation error and the local truncation error for the optimal and the usual method with function evaluation at three points.

Corollary 8: Let $f(x,y)$ have continuous derivatives with respect to y which satisfy $u_* \le \frac{\partial f}{\partial y} \le u^*$. Then the numerical solution $\{y_j\}$ of the difference equation

$$\hat{L}_2v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} -$$

$$\left\{\hat{\beta}_{0,i}f(x_{i-1},v_{i-1}) + \hat{\beta}_{1,i}f(x_i,v_i) + \hat{\beta}_{2,i}f(x_{i+1},v_{i+1})\right\},$$

and the solution $y(x)$ of the BVP (I) satisfy,

$$|y_j - y(x_j)| \le M \max_{1\le j\le N-1} |\hat{\tau}_j^2[y]|, \quad 0 \le j \le N,$$

where $\quad \hat{\tau}_j^2[\omega] \equiv \hat{L}_2\omega(x_j) - \mathcal{L}\omega(x_j), \quad 1 \le j \le N-1.$

Case 1 : $\quad -\infty < u^* < 0.$

$M = \hat{M}_3$, for all $h < \min\{H_3, H_4\}$, provided $\Phi h^2 \le \frac{1}{12}$.

Case 2: $\quad 0 < u^* < \pi^2/(b-a)^2.$

$M = \hat{M}_4$, for all $h < \min\ \{H_5, H_6\}$,

where $\hat{M}_3$, $\hat{M}_4$, H_3, H_4, H_5, H_6 are as given in Theorem 11.

Proof: From (I) and the definition of $\hat{L}_2$, evaluated at $x = x_j$, by the linearity of $\hat{L}_2$ and the Definition 15, as in Corollary 7, we get

$$\hat{L}_2[y_j - y(x_j)] = -\hat{\tau}_j^2\ [y].$$

Now since, $y_0 - y(x_0) = y_N - y(x_N) = 0$, applying Theorem 11, with $v_j - w_j = y_j - y(x_j)$, the result follows.

Corollary 9: Let $f(x,y)$ have continuous derivatives with respect to y which satisfy $u_* \le \frac{\partial f}{\partial y} \le u^*$. Then the numerical solution $\{y_j\}$ of the difference equation

$$L_2 v_i \equiv -\frac{v_{i-1} - 2v_i + v_{i+1}}{h^2} - \left\{\frac{1}{12} f(x_{i-1}, v_{i-1}) + \frac{10}{12} f(x_i, v_i) + \frac{1}{12} f(x_{i+1}, v_{i+1})\right\}$$

and the solution $y(x)$ of the BVP (I) satisfy,

$$|\ y_j - y(x_j)\ | \le M \max_{1 \le j \le N-1} |\tau_j^2\ [y]|, \quad 0 \le j \le N,$$

where $\quad \tau_j^2\ [\omega] \equiv L_2\omega(x_j) - \mathscr{L}\ \omega(x_j), \quad 1 \le j \le N-1.$

Case1 : $\quad -\infty < u^* < 0.$

$M = M_3$, for all $h < H_4$.

<u>Case 2:</u> $0 < u^* < \pi^2/(b-a)^2$.

with $M = M_4$, for all $h < \min\{H_6\ , H_7\}$,

where M_3, M_4, H_4, H_6, H_7 are as given in Proposition 2.

<u>Proof</u>: From (I) and the definition of L_2, evaluated at $x = x_j$, by the linearity of L_2 and the Definition 15, as in Corollary 7 we get

$$L_2[y_j - y(x_j)] = -\ \tau_j^2\ [y].$$

Now since, $y_0 - y(x_0) = y_N - y(x_N) = 0$, applying Theorem 11 with $v_j - w_j = y_j - y(x_j)$, the result follows.

CHAPTER - 4

OPTIMAL MULTISTEP METHODS IN $H^2(C_r)$ SPACE

4.1 Introduction

Quadrature formulae of various types with functions in space $H^2(C_r)$ have been discussed by Larkin [126]; Ritcher [157], [158], [159]; Chawla and Kaul [36], [37], [38]; Finney and Price Jr. [82]; Brij Bhusan [27] and others. Optimal multistep methods in this space for first order differential equations have been studied by Brij Bhusan [27]. In this chapter we shall study optimal multistep methods of various kinds discussed in Chapter 1, in the space $H^2(C_r)$, for the second order differential equations.

For the purpose of numerical illustration, as usual methods, we have taken Cowell's method with function evaluation at three points for both initial and boundary value problems, Stormer's method with function evaluation at five points in case of initial value problem only and Stormer's method with function evaluation at one point in case of boundary value problem only. We observe that the formulae obtained in this chapter are better suited for differential equations whose solutions have more pronounced singularities outside C_r but not too far from the boundary of C_r.

The norm in the space $H^2(C_r)$ is based on the line integral along the contour C_r. Hence the points in the neighbourhood of C_r get more weightage than the points inside C_r for the optimal multistep methods obtained in the space $H^2(C_r)$. So, the optimal methods in $H^2(C_r)$ space are more effective in the peripheral region

of the subinterval $[a,b]$ of $(-r,r)$.

In section 4.2, we prove that the second derivative of the kernel function of $H^2(C_r)$ space is the complex conjugate of the representer for the second derivative evaluation functional in $H^2(C_r)$. We devote section 4.3, for a discussion of optimal multistep methods in $H^2(C_r)$ and their numerical implementation; section 4.4, for a discussion of optimal multistep methods interpolatory for polynomials of certain degree and their numerical illustrations; section 4.5, for a discussion of optimal multistep methods interpolatory for certain other functions and their numerical illustrations. In section 4.6, we describe the limiting behaviour of the optimal coefficients as $r \to \infty$. In section 4.7, we are calculating and comparing the asymptotic behaviour of the local truncation error (LTE) functionals for usual and the β-optimal methods in $H^2(C_r)$ space.

4.2 The Hilbert space $H^2(C_r)$

The space $H^2(C_r)$ consists of functions of a complex variable z which are analytic within the disc $D_r = \{z : |z| < r\}$ and square integrable on the circle $C_r = \{z : |z| = r\}$. The space $H^2(C_r)$ is a Hilbert space with the inner product defined by

$$(1) \qquad (f,g) = \int_{C_r} f(z)\,\overline{g(z)}\,ds, \qquad f,\ g \in H^2(C_r),$$

the integration being with respect to the length element ds on the circle.

This space possesses a reproducing kernel function given by

(2) $$K(z,\overline{t}) = \frac{r}{2\pi(r^2 - z\overline{t})}$$

and a complete orthonormal sequence $\{\psi_k\}$ of functions (Szegő [177])

(3) $$\psi_k(z) = \frac{z^k}{\sqrt{2\pi r}\, r^k}, \qquad k = 0,1,2,\ldots\ldots .$$

As the space $H^2(C_r)$ possesses a reproducing kernel function, the linear functional for point evaluation

$$L_z : f \longrightarrow f(z), \qquad f \in H^2(C_r),\ z \in D_r$$

is a bounded linear functional (Aronszajn [4]).

Also the representer of k-th derivative evaluation functional

$$Dk(z) : f \longrightarrow f^k(z); \qquad f \in H^2(C_r),\ z \in D_r,$$

where k is a positive integer, is a bounded linear functional and with a bound given as follows.

<u>Theorem 1:</u> (Brij Bhusan [27]) For $z \in D_r$ and k any positive integer, $Dk(z)$ is a bounded linear functional in $H^2(C_r)$ with

$$\| D_z^k \| \leq \frac{k!\sqrt{r}}{\sqrt{2\pi}(r-|z|)^{k+1}} .$$

The representer $D2(t,\overline{z}_0)$ of the second derivative evaluation functional at a point $z_0 \in D_r$, should satisfy

$$D2(t,\overline{z}_0) = \overline{\frac{\partial^2}{\partial z^2} K(z,\overline{t})}\Big|_{z=z_0} = \frac{rt^2}{\pi(r^2-\overline{z}_0 t)^3}.$$

<u>Theorem 2:</u> The function

$$D2(t,\overline{z}_0) = \frac{rt^2}{\pi(r^2-\overline{z}_0 t)^3}$$

is the representer for the 2-nd derivative evaluation functional at $z_0 \in D_r$.

<u>Proof:</u> The only singularity of $D2(t,\bar{z}_0)$ is a pole of order 3 at $t = \frac{r^2}{\bar{z}_0}$. As $z_0 \in D_r$, $\frac{r^2}{\bar{z}_0}$ lies outside C_r. Hence the function $D2(t,\bar{z}_0)$ belongs to $H^2(C_r)$. Now we have to show that

$$f''(z_0) = \left(f(t) \;,\; \frac{rt^2}{\pi(r^2-\bar{z}_0 t)^3}\right).$$

By Cauchy integral formula

$$\begin{aligned}
f''(z_0) &= \frac{2!}{2\pi i}\int_{C_r} \frac{f(t)}{(t-z_0)^3}\,dt \\
&= \frac{1}{\pi i}\int_0^{2\pi} \frac{f(t)}{(re^{i\theta}-z_0)^3}\, re^{i\theta}\, i\, d\theta, \qquad \text{putting } t = re^{i\theta} \\
&= \frac{r}{\pi}\int_0^{2\pi} \frac{f(t)r^2e^{-2i\theta}}{(re^{i\theta}-z_0)^3 r^3 e^{-3i\theta}}\, r d\theta \\
&= \int_{C_r} f(t)\, \overline{\left\{\frac{r}{\pi}\,\frac{(re^{i\theta})^2}{(r^2-\bar{z}_0 re^{i\theta})^3}\right\}}\, ds \\
&= \left(f(t) \;,\; \frac{r}{\pi}\,\frac{t^2}{(r^2-\bar{z}_0 t)^3} \right),
\end{aligned}$$

which proves the result.

In $H^2(C_r)$ space we have the following :

(4) $$K(z,\bar{t}) = \frac{r}{2\pi(r^2-z\bar{t})}$$

(5) $$D2(t,\bar{z}) = \overline{\frac{\partial^2}{\partial z^2} K(z,\bar{t})} = \frac{rt^2}{\pi(r^2-t\bar{z})^3}$$

(6) $$D2''(t,\bar{z}) = \frac{\partial^2}{\partial t^2} D2(t,\bar{z}) = \frac{r}{\pi}\,\frac{2}{(r^2-t\bar{z})^3}\left[1 + \frac{6t\bar{z}}{(r^2-t\bar{z})} + \frac{6t^2\bar{z}^2}{(r^2-t\bar{z})^2}\right]$$

Now we shall implement in $H^2(C_r)$ space, (i) β-optimal method, (ii) α-optimal method, (iii) β-optimal method with restriction, (iv) β-optimal method interpolatory for polynomials, and (v)

β-optimal method interpolatory for linearly independent functions exp(1.6x) and exp(-1.6x), on twenty four BVP's and twenty four IVP's with differential equations listed below, using Cowell's method with function evaluation at three points as the usual mehod in which $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=1/12$, $\beta_1=10/12$, and $\beta_2=1/12$. We also implement (vi) β-optimal method, on twenty four BVP's using Stormer's method with function evaluation at one point as the usual method in which $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_1=1$, and (vii) β-optimal method, on twenty four IVP's using Stormer's explicit method with function evaluation at five points as the usual method in which $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=299/240$, $\beta_1=-11/15$, $\beta_2=97/120$, $\beta_3= -2/5$, and $\beta_4=19/240$. The initial values for the IVP's and the boundary values for the BVP's are calculated from the analytical solutions. Tables for optimal beta coefficients are common for BVP-s and IVP-s if the differential equation is written in the common form $y'' = f(x,y)$. Throughout this thesis, the numerical experiments are done with this convention. The Key symbols used in the following tables are as follows:

r-sum : row sum of $\hat{\beta}_{i,n}$'s,

$\|T_n\|^2$: square norm of LTE functional for usual method,

$\|\hat{T}_n\|^2$: square norm of LTE functional for optimal method,

itu : number of iterations for convergence of the solution using usual method,

ito : number of iterations for convergence of the solution using optimal method,

$\bar{e}_u$: average of absolute values of point wise discretisation errors for usual method,

$\bar{e}_o$: average of absolute values of point wise discretisation errors for optimal method.

The twenty four differential equations and their analytical (particular) solutions are listed below.

1. $\frac{d^2y}{dx^2} = y^3(1 + 3x^2y^2)$; $y = (2.01^2 - x^2)^{-1/2}$.

2. $\frac{d^2y}{dx^2} = y^3(1 + 3x^2y^2)$; $y = (2.11^2 - x^2)^{-1/2}$.

3. $\frac{d^2y}{dx^2} = 2y^2(1 + 4x^2y)$; $y = (2.03^2 - x^2)^{-1}$.

4. $\frac{d^2y}{dx^2} = 2y^2(1 + 4x^2y)$; $y = (2.11^2 - x^2)^{-1}$.

5. $\frac{d^2y}{dx^2} = - 2e^{-y}(1 + 2x^2e^{-y})$; $y = \log(2.01^2 - x^2)$.

6. $\frac{d^2y}{dx^2} = 4x^2y^2(3 + 8x^4y)$; $y = (2.01^4 - x^4)^{-1}$.

7. $\frac{d^2y}{dx^2} = 6x^4y^2(5 + 12x^6y)$; $y = (2.01^6 - x^6)^{-1}$.

8. $\frac{d^2y}{dx^2} = 6x^2y^3(1 + 2x^4y^2)$; $y = (2.01^4 - x^4)^{-1/2}$.

9. $\frac{d^2y}{dx^2} = 3x^4y^3(5 + 9x^6y^2)$; $y = (2.01^6 - x^6)^{-1/2}$.

10. $\frac{d^2y}{dx^2} = 2y(1 + 2x^2)$; $y = e^{x^2}$.

11. $\frac{d^2y}{dx^2} = 9y$; $y = \cosh(3x)$.

12. $\frac{d^2y}{dx^2} = 9y$; $y = \sinh(3x)$.

13. $\frac{d^2y}{dx^2} = y^3(1 + 3x^2y^2)$; $y = (2.75^2 - x^2)^{-1/2}$.

14. $\frac{d^2y}{dx^2} = y^3(1 + 3x^2y^2)$; $y = (2.85^2 - x^2)^{-1/2}$.

15. $\frac{d^2y}{dx^2} = 2y^2(1 + 4x^2y)$; $y = (2.77^2 - x^2)^{-1}$.

16. $\dfrac{d^2y}{dx^2} = 2y^2(1 + 4x^2y)$; $\quad y = (2.85^2 - x^2)^{-1}$.

17. $\dfrac{d^2y}{dx^2} = 6x^4y^2(5 + 12x^6y)$; $\quad y = (2.85^6 - x^6)^{-1}$.

18. $\dfrac{d^2y}{dx^2} = 3x^4y^3(5 + 9x^6y^2)$; $\quad y = (2.9^6 - x^6)^{-1/2}$.

19. $\dfrac{d^2y}{dx^2} = -\dfrac{4y(1 + 6x^2y)}{x^2+0.9} + \dfrac{24x^2y}{(x^2+0.9)^2} + 2y^2(1 + 4x^2y)$;

$$y = (2.02^2 - x^2)^{-1} + (x^2 + 0.9)^{-1}.$$

20. $\dfrac{d^2y}{dx^2} = 2y^2(2x^2 - 3.1804) + 8x^2y^3(2x^2 - 3.1804)^2 + 8x^2y^2$;

$$y = (2.02^2 - x^2)^{-1}(x^2 + 0.9)^{-1}.$$

21. $\dfrac{d^2y}{dx^2} = y^3(2x^2 - 3.1804) + 3x^2y^5(2x^2 - 3.1804)^2 + 4x^2y^3$;

$$y = (2.02^2-x^2)^{-1/2}(x^2+0.9)^{-1/2}.$$

22. $\dfrac{d^2y}{dx^2} = y^3(1+3x^2y^2) - \dfrac{3y^2(1+ 5x^2y^2)}{(x^2 +0.9)^{1/2}} + \dfrac{3y(1+10x^2y^2)}{x^2+0.9} - \dfrac{2(1+15x^2y^2)}{(x^2+0.9)^{3/2}}$

$+ \dfrac{15x^2y}{(x^2 + 0.9)^2}$; $\quad y = (2.02^2-x^2)^{-1/2} + (x^2+0.9)^{-1/2}$.

23. $\dfrac{d^2y}{dx^2} = -\dfrac{2(e^{-y} + 1)}{x^2 + 0.9} + \dfrac{4x^2(1 - e^{-2y})}{(x^2 + 0.9)^2}$; $\quad y = \log\left(\dfrac{2.02 - x^2}{x^2 + 0.9}\right)^2$.

24. $\dfrac{d^2y}{dx^2} = 27x^{10}y^5(x^2+0.9)^4 + 15x^4y^3(x^2+0.9)^2 - 12x^6y^3(x^2+0.9)$

$- \dfrac{2y}{x^2+0.9} + \dfrac{8x^2y}{(x^2+0.9)^2}$; $\quad y = \dfrac{(2.02^6-x^6)^{-1/2}}{x^2+0.9}$.

The equations 1-9 have solutions with singularities of various kinds near the boundary of the domain of $H^2(C_r)$ space with r=2.01. The solutions of equations 10-12 are entire functions of fast growth. The equations 13-18 have solutions with singularities near

the boundary of the domain of $H^2(C_r)$ space with r=2.8. The equations 19-24 have solutions with singularities inside the domain of the space $H^2(C_r)$ with r=2.01.

4.3 Optimal Multistep Methods in $H^2(C_r)$-Space

In $H^2(C_r)$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$ of β-optimal multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} f_{n+k-j} = 0 \tag{7}$$

where α_j's are prefixed according to some consistent and stable known usual method with highest degree polynomial precision,

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0, \tag{8}$$

with reference to equation (11) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where $\hat{b} = h^2\left(\hat{\beta}_{\delta_{t0},n}, \ldots\ldots\ldots, \hat{\beta}_{k,n}\right)^T$,

$$\hat{c}_{ij} = \frac{r}{\pi}\,\frac{2}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^3}\left[1 + \frac{6x_{n+k-j}\bar{x}_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})} + \frac{6x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}\right],$$

for $i,j = \delta_{t0}(1)k$,

$$\hat{d}_i = -\frac{r}{\pi}\sum_{j=0}^{k}\alpha_j\,\frac{x^2_{n+k-j}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^3}, \quad i = \delta_{t0}(1)k.$$

This system of equations may be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{t0}(1)k$.

The following theorem characterizes the β-optimal multistep method (7) in $H^2(C_r)$ space.

<u>Theorem 3:</u> The optimal multistep method (7) in which α_j's are prefixed, and optimization is done with respect to β_j's in $H^2(C_r)$ space is characterized by that it is locally interpolatory for functions

$$\left\{ y_i(x) = \frac{x^2}{(r^2 - x\bar{x}_{n+k-i})^3},\ i = \delta_{t0}(1)k \right\}.$$

<u>Proof:</u> The proof follows from Theorem 1 of Chapter 1, using (4) (5) and (6), the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$.

<u>Corollary 1:</u> If $x_{n+k-i} = 0$, for some $i = \delta_{t0}(1)k$ then the optimal method (7) becomes consistent.

<u>Proof:</u> Since the corresponding usual formula (8) is consistent, we have $\sum_{j=0}^{k} \alpha_j = 0$, $\sum_{j=0}^{k} j\alpha_j = 0$; which also holds for the β-optimal method (7). In other words, the optimal method (7) is exact for constants and $y(x) = x$. Furthermore, if $x_{n+k-i} = 0$, for some $i = \delta_{t0}(1)k$, then by Theorem 3, the optimal method (7) is exact for $y(x) = x^2$. Hence the optimal method (7) is consistent.

In the following tables we are presenting the numerical results for various optimal methods.

Table - 1a

x_n	$h^2\hat{\beta}_{1n}$	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.1064E-01	.4190E-04	.2339E-04
-1.6	.1035E-01	.3253E-05	.1846E-05
-1.5	.1022E-01	.4566E-06	.2677E-06
-1.4	.1015E-01	.9279E-07	.5665E-07
-1.3	.1010E-01	.2433E-07	.1553E-07
-1.2	.1008E-01	.7695E-08	.5154E-08
-1.1	.1006E-01	.2811E-08	.1979E-08
-1.0	.1004E-01	.1153E-08	.8546E-09
-.9	.1003E-01	.5201E-09	.4062E-09
-.8	.1002E-01	.2546E-09	.2093E-09
-.7	.1002E-01	.1339E-09	.1157E-09
-.6	.1001E-01	.7532E-10	.6807E-10
-.5	.1001E-01	.4518E-10	.4245E-10
-.4	.1001E-01	.2899E-10	.2807E-10
-.3	.1000E-01	.2004E-10	.1979E-10
-.2	.1000E-01	.1512E-10	.1507E-10
-.1	.1000E-01	.1264E-10	.1264E-10
.0	.1000E-01	.1189E-10	.1189E-10
.1	.1000E-01	.1264E-10	.1264E-10
.2	.1000E-01	.1512E-10	.1507E-10
.3	.1000E-01	.2004E-10	.1979E-10
.4	.1001E-01	.2899E-10	.2807E-10
.5	.1001E-01	.4518E-10	.4245E-10
.6	.1001E-01	.7532E-10	.6807E-10
.7	.1002E-01	.1339E-09	.1157E-09
.8	.1002E-01	.2546E-09	.2093E-09
.9	.1003E-01	.5201E-09	.4062E-09
1.0	.1004E-01	.1153E-08	.8546E-09
1.1	.1006E-01	.2811E-08	.1979E-08
1.2	.1008E-01	.7695E-08	.5154E-08
1.3	.1010E-01	.2433E-07	.1553E-07
1.4	.1015E-01	.9279E-07	.5665E-07
1.5	.1022E-01	.4566E-06	.2677E-06
1.6	.1035E-01	.3253E-05	.1846E-05
1.7	.1064E-01	.4190E-04	.2339E-04

Optimal β and the square norm of local truncation error functionals for 1-point Stormer's usual and β-optimal methods in $H^2(C_r)$ -space, for 24 BVP-s, with r=2.01, a=-1.8, b=1.8, n=36, h=.1, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_1=1$.

The above table shows that numerically $\hat{\beta}_{1n}$'s are dependent on points. At a point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$, and in a neighbourhood of the origin, $\hat{\beta}_1$'s are close to usual β_1, $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are very close.

Table - 1b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	3	.275334E-02	3	.745402E-03
2	3	.137251E-02	2	.131767E-03
3	3	.425201E-02	3	.171838E-02
4	3	.226162E-02	2	.393388E-03
5	3	.547598E-02	2	.391630E-03
6	3	.110208E-02	3	.512200E-03
7	3	.269263E-03	3	.127965E-03
8	3	.152372E-02	3	.451638E-03
9	3	.829285E-03	3	.275791E-03
10	1	.122695E+00	1	.897968E-01
11	1	.163739E+00	1	.715156E-01
12	1	.159277E+00	1	.678948E-01
13	2	.262515E-03	2	.116181E-03
14	2	.190524E-03	2	.655540E-04
15	2	.279694E-03	2	.158166E-03
16	2	.207536E-03	2	.104474E-03
17	2	.237192E-05	2	.143541E-05
18	2	.200635E-04	2	.108095E-04
19	3	.486991E-02	3	.191473E-02
20	4	.601963E-02	3	.295464E-02
21	3	.473819E-02	3	.151276E-02
22	3	.268350E-02	3	.558582E-03
23	3	.474838E-02	2	.856693E-03
24	3	.924705E-03	2	.320007E-03

Table for number of iterations for convergence of the solution and the average discretisation error using Stormer's 1-point usual and β-optimal methods in $H^2(C_r)$-space, for 24 BVP-s.

The results in Table-1b are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1 for the equations 1-9, 18-24; and with r=2.8, a=-2.1, b=2.1, n=42, h=.1 for the equations 10-18. The optimal method is one decimal place better on equations 1,2,4-6,8,10-12, 14,22,23; and just better on equations 3,7,9,13,15-18,19,20,21,24.

Table - 2a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.6405E-03	.9069E-02	.1461E-03	.9855E-02	.1102E-05	.9991E-07
-1.6	.7134E-03	.8720E-02	.5246E-03	.9958E-02	.2478E-07	.2731E-08
-1.5	.7530E-03	.8567E-02	.6637E-03	.9984E-02	.1375E-08	.1808E-09
-1.4	.7770E-03	.8487E-02	.7292E-03	.9993E-02	.1326E-09	.2075E-10
-1.3	.7926E-03	.8439E-02	.7650E-03	.9996E-02	.1860E-10	.3476E-11
-1.2	.8033E-03	.8408E-02	.7866E-03	.9998E-02	.3431E-11	.7689E-12
-1.1	.8109E-03	.8387E-02	.8006E-03	.9999E-02	.7802E-12	.2106E-12
-1.0	.8166E-03	.8373E-02	.8101E-03	.9999E-02	.2094E-12	.6830E-13
-.9	.8209E-03	.8362E-02	.8168E-03	.1000E-01	.6440E-13	.2536E-13
-.8	.8242E-03	.8354E-02	.8217E-03	.1000E-01	.2219E-13	.1050E-13
-.7	.8267E-03	.8348E-02	.8253E-03	.1000E-01	.8485E-14	.4806E-14
-.6	.8287E-03	.8343E-02	.8279E-03	.1000E-01	.3576E-14	.2396E-14
-.5	.8303E-03	.8340E-02	.8298E-03	.1000E-01	.1626E-14	.1254E-14
-.4	.8314E-03	.8337E-02	.8312E-03	.1000E-01	.8270E-15	.7184E-15
-.3	.8323E-03	.8336E-02	.8322E-03	.1000E-01	.4759E-15	.4490E-15
-.2	.8329E-03	.8334E-02	.8328E-03	.1000E-01	.2995E-15	.2949E-15
-.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.2026E-15	.2023E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.1766E-15	.1766E-15
.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.1319E-15	.1316E-15
.2	.8328E-03	.8334E-02	.8329E-03	.1000E-01	.2288E-15	.2242E-15
.3	.8322E-03	.8336E-02	.8323E-03	.1000E-01	.4405E-15	.4137E-15
.4	.8312E-03	.8337E-02	.8314E-03	.1000E-01	.8094E-15	.7008E-15
.5	.8298E-03	.8340E-02	.8303E-03	.1000E-01	.1608E-14	.1236E-14
.6	.8279E-03	.8343E-02	.8287E-03	.1000E-01	.3523E-14	.2342E-14
.7	.8253E-03	.8348E-02	.8267E-03	.1000E-01	.8555E-14	.4877E-14
.8	.8217E-03	.8354E-02	.8242E-03	.1000E-01	.2230E-13	.1061E-13
.9	.8168E-03	.8362E-02	.8209E-03	.1000E-01	.6440E-13	.2536E-13
1.0	.8101E-03	.8373E-02	.8166E-03	.9999E-02	.2094E-12	.6825E-13
1.1	.8006E-03	.8387E-02	.8109E-03	.9999E-02	.7802E-12	.2106E-12
1.2	.7866E-03	.8408E-02	.8033E-03	.9998E-02	.3431E-11	.7690E-12
1.3	.7650E-03	.8439E-02	.7926E-03	.9996E-02	.1860E-10	.3476E-11
1.4	.7292E-03	.8487E-02	.7770E-03	.9993E-02	.1326E-09	.2075E-10
1.5	.6637E-03	.8567E-02	.7530E-03	.9984E-02	.1375E-08	.1808E-09
1.6	.5246E-03	.8720E-02	.7134E-03	.9958E-02	.2478E-07	.2731E-08
1.7	.1461E-03	.9069E-02	.6405E-03	.9855E-02	.1102E-05	.9991E-07

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using 3-points Cowell's usual and the corresponding β-optimal methods in $H^2(C_r)$ -space, at the nodal points, with a=-1.8, b=1.8, n=36, h=.1, r=2.01 α_0=-1, α_1=2, α_2=-1, β_0=.083333, β_1=.833333, β_2=.083333.

From Table 2a, it is seen that $\hat{\beta}_i$'s are dependent on points, in a neighbourhood of the origin they are very close to usual β_i's. At a general point x_n, $\|\hat{T}_n\|^2 \leq \|T_n\|^2$ and in a neighbourhood of the

origin $x_n=0$, $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are nearly equal.

In the list of 24 differential equations, various equations need various ranges of intervals for the optimal methods to show better performance than the usual method. For convenience of presentation in tabular form we compromise in this regard. We take a common domain of the space $H^2(C_r)$ and the interval of IVP or BVP for a class of differential equations for each of which the optimal methods perform just better or better than the usual method. The exceptional cases are discussed separately.

In Table 2b(i) we present the numerical results obtained from 24 BVP's in $H^2(C_r)$-space with r=2.01 a=-1.8, b=1.8, n=36, h=.1. The optimal method produces worse results than the usual method while implemented on the equations 10-18. This phenomena happens because the solutions of the equations 10-12 are entire functions and the solutions of the equations 13-18 have singularities far from the boundary of the domain of $H^2(C_r)$-space with r=2.01. However, with increasing domain of the space $H^2(C_r)$ and with increasing interval [a,b] viz. with r=2.8 a=-2.1, b=2.1, n=42, h=.1, β- optimal method performs better than the usual method and these results are shown in Table 2b(ii). Similar cause and effect are also observed in other optimal methods discussed latter. Tables 2b(i) and 2b(ii) reveal that as compared to the usual method, the β-optimal method for BVP is two decimal places better on equations 4, 21, 22; one decimal place better on equations 1,3,5-14,16-20,23; and just better on equations 2,15,24.

Table - 2b(i)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.156144E-04
2	2	.610703E-04	2	.178799E-04
3	3	.430195E-03	2	.479332E-04
4	2	.133292E-03	2	.657091E-05
5	2	.348263E-03	2	.659629E-04
6	3	.127772E-03	2	.198516E-04
7	2	.313175E-04	2	.511442E-05
8	2	.133523E-03	2	.104334E-04
9	2	.735570E-04	2	.794383E-05
10	1	.506252E-03	1	.392665E-03
11	1	.351768E-03	1	.459791E-02
12	1	.331492E-03	1	.453892E-02
13	2	.698086E-06	2	.165936E-04
14	2	.451879E-06	2	.152147E-04
15	2	.869978E-06	2	.113683E-04
16	2	.592198E-06	2	.104150E-04
17	1	.544969E-08	1	.321212E-07
18	1	.382493E-07	1	.344680E-06
19	3	.509406E-03	2	.496179E-04
20	3	.464907E-03	2	.452461E-04
21	2	.304135E-03	2	.292641E-05
22	2	.208304E-03	2	.616719E-05
23	2	.300455E-03	2	.758440E-04
24	2	.287372E-04	2	.173342E-04

Table - 2b(ii)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
10	1	.170782E-02	1	.246413E-03
11	1	.738872E-03	1	.659951E-04
12	1	.718937E-03	1	.566636E-04
13	2	.298705E-05	2	.553934E-06
14	2	.167071E-05	1	.121468E-06
15	2	.392662E-05	2	.103090E-05
16	2	.236517E-05	2	.469570E-06
17	1	.257920E-07	1	.793687E-08
18	1	.151826E-06	1	.478944E-07

Tables for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods in $H^2(C_r)$-space, for 24 BVP-s.

Table - 2c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.967316E-03
2	4	.250457E-02	3	.554172E-03
3	8	.760039E-01	5	.797436E-02
4	5	.132805E-01	3	.154057E-03
5	4	.716823E-02	4	.139008E-02
6	5	.356402E-02	4	.585207E-03
7	4	.354625E-03	3	.650670E-04
8	4	.211573E-02	3	.185227E-03
9	3	.604542E-03	3	.843654E-04
10	4	.119641E-01	4	.577624E-02
11	4	.130464E+00	4	.159482E-01
12	4	.129361E+00	4	.158529E-01
13	2	.128426E-05	1	.249427E-06
14	2	.831124E-06	1	.817898E-07
15	2	.193794E-05	2	.612107E-06
16	2	.130401E-05	2	.344920E-06
17	1	.456442E-08	1	.932196E-09
18	1	.343343E-07	1	.276732E-08
19	11	.103867E+00	5	.520553E-02
20	4	.188589E-02	3	.128487E-03
21	4	.112364E-02	3	.630115E-04
22	5	.115497E-01	4	.746171E-03
23	4	.610397E-02	3	.112045E-02
24	3	.542588E-04	3	.660853E-04

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods in $H^2(C_r)$-space, for 24 IVP-s.

In Table 2c, we present the numerical results on 24 IVP's. The performance of the optimal method on the IVP's 10-18 is the same as in Table 2b. So, for IVP's 1-9 and 19-24 we take r=2.01, a=-1.7, b=1.7, n=34, h=.1; and for the IVP's 10-18 we take r=2.7, a=-1.4, b=1.4, n=28, h=.1. Still for the IVP 24, the optimal method is giving little worse result compared to the usual method in the interval a=-1.7, b=1.7. But with an increasing interval, say a=-1.8, b=1.8 and with r=2.01, n=36, h=.1, the optimal method for IVP 24 gives just better result compared to the usual method, given by itu=24, $\bar{e}_u$=.404924E-03, ito=3, $\bar{e}_o$=.200161E-03.

From Table 2c, we see that as compared to the usual method, the β-optimal method for IVP is two decimal places better on equations 1,4,19,21,22; one decimal place better on equations 2,3, 6-18,20; and just better on equations 5,23,24.

Table - 3a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	$h^2\hat{\beta}_{3n}$	$h^2\hat{\beta}_{4n}$
-1.3	.1014E-01	-.6255E-03	.5450E-03	-.9355E-04	.5185E-05
-1.2	.1045E-01	-.1234E-02	.9636E-03	-.2122E-03	.1663E-04
-1.1	.1071E-01	-.1811E-02	.1426E-02	-.3695E-03	.3560E-04
-1.0	.1093E-01	-.2350E-02	.1908E-02	-.5550E-03	.6152E-04
-.9	.1112E-01	-.2851E-02	.2394E-02	-.7610E-03	.9346E-04
-.8	.1129E-01	-.3319E-02	.2879E-02	-.9815E-03	.1305E-03
-.7	.1144E-01	-.3756E-02	.3359E-02	-.1213E-02	.1719E-03
-.6	.1157E-01	-.4167E-02	.3830E-02	-.1452E-02	.2169E-03
-.5	.1169E-01	-.4556E-02	.4294E-02	-.1697E-02	.2652E-03
-.4	.1180E-01	-.4925E-02	.4751E-02	-.1947E-02	.3166E-03
-.3	.1191E-01	-.5280E-02	.5205E-02	-.2204E-02	.3709E-03
-.2	.1201E-01	-.5624E-02	.5657E-02	-.2468E-02	.4286E-03
-.1	.1210E-01	-.5962E-02	.6114E-02	-.2742E-02	.4901E-03
.0	.1219E-01	-.6298E-02	.6579E-02	-.3028E-02	.5560E-03
.1	.1228E-01	-.6637E-02	.7058E-02	-.3330E-02	.6273E-03
.2	.1237E-01	-.6982E-02	.7559E-02	-.3653E-02	.7053E-03
.3	.1246E-01	-.7340E-02	.8090E-02	-.4002E-02	.7917E-03
.4	.1255E-01	-.7716E-02	.8660E-02	-.4387E-02	.8889E-03
.5	.1265E-01	-.8117E-02	.9283E-02	-.4816E-02	.9999E-03
.6	.1275E-01	-.8553E-02	.9975E-02	-.5304E-02	.1129E-02
.7	.1286E-01	-.9035E-02	.1076E-01	-.5870E-02	.1282E-02
.8	.1299E-01	-.9577E-02	.1166E-01	-.6540E-02	.1468E-02
.9	.1312E-01	-.1020E-01	.1273E-01	-.7354E-02	.1700E-02
1.0	.1328E-01	-.1094E-01	.1403E-01	-.8369E-02	.1997E-02
1.1	.1346E-01	-.1182E-01	.1565E-01	-.9676E-02	.2392E-02
1.2	.1368E-01	-.1292E-01	.1773E-01	-.1142E-01	.2938E-02
1.3	.1394E-01	-.1434E-01	.2053E-01	-.1386E-01	.3732E-02
1.4	.1428E-01	-.1624E-01	.2447E-01	-.1746E-01	.4956E-02
1.5	.1473E-01	-.1893E-01	.3040E-01	-.2319E-01	.7004E-02
1.6	.1537E-01	-.2306E-01	.4017E-01	-.3327E-01	.1084E-01
1.7	.1636E-01	-.3013E-01	.5859E-01	-.5396E-01	.1933E-01
1.8	.1810E-01	-.4470E-01	.1018E+00	-.1083E+00	.4393E-01

Table for optimal β's in $H^2(C_r)$-space using β-optimal method corresponding to Stormer's 5-points explicit method , with r=2.01, a=-1.8, b=1.8, n=36, h=.1, α_0=-1, α_1=2, α_2=-1, β_0=1.2458, β_1=-.73333, β_2=.80833, β_3=-.4, β_4=.079167.

Table - 3b

x	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.200	.422951E-06	.204586E-10
-1.100	.285004E-07	.441966E-11
-1.000	.303227E-08	.122238E-11
-.900	.444703E-09	.414708E-12
-.800	.829548E-10	.166763E-12
-.700	.186873E-10	.773688E-13
-.600	.490718E-11	.406314E-13
-.500	.146524E-11	.237813E-13
-.400	.488836E-12	.153025E-13
-.300	.180134E-12	.107809E-13
-.200	.729000E-13	.825421E-14
-.100	.324572E-13	.681878E-14
.000	.161350E-13	.605826E-14
.100	.934011E-14	.581015E-14
.200	.671864E-14	.593563E-14
.300	.663617E-14	.663170E-14
.400	.895454E-14	.800753E-14
.500	.151874E-13	.103936E-13
.600	.301961E-13	.146960E-13
.700	.670408E-13	.225418E-13
.800	.164070E-12	.381147E-13
.900	.440959E-12	.717456E-13
1.000	.130761E-11	.152142E-12
1.100	.432537E-11	.369664E-12
1.200	.162302E-10	.105397E-11
1.300	.707462E-10	.364126E-11
1.400	.370494E-09	.159507E-10
1.500	.244802E-08	.946202E-10
1.600	.219908E-07	.840254E-09
1.700	.303696E-06	.131715E-07

Table for square norm of local truncation error functionals in $H^2(C_r)$-space, for Stormer's 5-points explicit method and the corresponding β-optimal method at the nodal points, with r=2.01, a=-1.7, b=1.7, n=34, h=.1.

From Table 3a, it is seen that the optimal coefficients $\hat{\beta}_{in}$, i = 0(1)4 are varying from point to point and at a neighbourhood of x=0, they are close to the usual coefficients β_i, i = 0(1)4.

Table 3b, displays that at a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$ and at the beginning and the end of the table, the ratios of $\|\hat{T}_n\|^2$ to $\|T_n\|^2$ are much less than that at the middle of the table.

Table - 3c

eqn.	$\bar{e}_u$	$\bar{e}_0$
1	.304356E-01	.390952E-04
2	.632144E-02	.655918E-04
3	.167084E+00	.987157E-04
4	.289167E-01	.611449E-04
5	.186264E-01	.252343E-03
6	.748945E-02	.210860E-04
7	.854658E-03	.302262E-05
8	.515672E-02	.162121E-04
9	.163408E-02	.659739E-05
10	.402219E+02	.838737E-02
11	.670431E+02	.633130E+00
12	.670732E+02	.503651E+00
13	.635226E-03	.170320E-05
14	.266670E-03	.242168E-05
15	.152962E-02	.141532E-04
16	.700262E-03	.243861E-05
17	.148635E-05	.104435E-07
18	.672210E-05	.343957E-08
19	.246038E+00	.342962E-03
20	.415804E-02	.202398E-04
21	.282785E-02	.369438E-04
22	.253443E-01	.332677E-03
23	.161435E-01	.118800E-02
24	.151126E-03	.115419E-04

Table for number of iterations for convergence of the solution and the average discretisation error using Stormer's 5-points usual and the corresponding β-optimal methods in $H^2(C_r)$-space, for 24 IVP-s.

In Table 3c, the results for IVP's with equations 1-9 and 19-24 are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1; and for IVP's with equations 10-18 are obtained with r=2.8, a=-2.1, b=2.1, n=42, h=.1. As compared to usual method, the β-optimal method for IVP is four decimal places better on equations 3,10; three decimal places better on equations 1,4,9,18,19; two decimal places better on equations 2,5-8,11-17,20-22; and one decimal place better on equations 23,24.

In $H^2(C_r)$ space, to determine the optimal coefficients $\hat{\alpha}_{i,n}$, i = 0(1)k of an α -optimal multistep method

$$(9) \qquad \sum_{j=0}^{k} \hat{\alpha}_{j,n} y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0,$$

where β_j's are prefixed according to some consistent and stable known usual method with highest degree polynomial precision. With reference to equation (13) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{a} = \hat{d},$$

where $\hat{a} = \left(\hat{\alpha}_{0,n}, \ldots\ldots, \hat{\alpha}_{k,n}\right)^T$,

$$\hat{c}_{ij} = \frac{r}{2\pi} \frac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})}, \qquad i,\ j = 0(1)k, \quad \text{and}$$

$$\hat{d}_i = -\frac{r}{\pi} h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \frac{\bar{x}^2_{n+k-i}}{(r^2 - \bar{x}_{n+k-i} x_{n+k-j})^3}, \qquad i = 0(1)k.$$

This system of equations can be solved for $\hat{\alpha}_{j,n}$, j = 0(1)k.

The following theorem characterizes the α-optimal multistep method (9) in $H^2(C_r)$ space.

<u>Theorem 4:</u> The α-optimal multistep method (9) in which β_j's are prefixed and optimization is done with respect to α_j's in $H^2(C_r)$space, is characterized by that it is locally interpolatory for functions

$$\left\{ y_i(x) = \frac{1}{(r^2 - x\bar{x}_{n+k-i})},\ i = 0(1)k \right\}.$$

<u>Proof:</u> The proof follows from Theorem 2 of Chapter 1, using the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

Remark: If $x_{n+k-i} = 0$, for some $i = 0(1)k$, then the α-optimal method (9) is locally interpolatory for constants, which in other words tells that $\sum_{j=0}^{k} \hat{\alpha}_{j,n} = 0$.

Table - 4a

x_n	$\hat{\alpha}_{0n}$	$\hat{\alpha}_{1n}$	$\hat{\alpha}_{2n}$	r-sum	$\lVert T_n \rVert^2$	$\lVert \hat{T}_n \rVert^2$
-1.5	-.1000E+01	.2001E+01	-.1001E+01	-.3515E-05	.1629E-09	.1441E-09
-1.4	-.1000E+01	.2001E+01	-.1000E+01	-.1078E-05	.2208E-10	.2007E-10
-1.3	-.1000E+01	.2000E+01	-.1000E+01	-.3659E-06	.3966E-11	.3687E-11
-1.2	-.1000E+01	.2000E+01	-.1000E+01	-.1328E-06	.8822E-12	.8363E-12
-1.1	-.1000E+01	.2000E+01	-.1000E+01	-.5014E-07	.2323E-12	.2239E-12
-1.0	-.1000E+01	.2000E+01	-.1000E+01	-.1926E-07	.7020E-13	.6847E-13
-.9	-.1000E+01	.2000E+01	-.1000E+01	-.7369E-08	.2378E-13	.2337E-13
-.8	-.1000E+01	.2000E+01	-.1000E+01	-.2747E-08	.8889E-14	.8876E-14
-.7	-.1000E+01	.2000E+01	-.1000E+01	-.9720E-09	.3630E-14	.3688E-14
-.6	-.1000E+01	.2000E+01	-.1000E+01	-.3154E-09	.1623E-14	.1655E-14
-.5	-.1000E+01	.2000E+01	-.1000E+01	-.8929E-10	.7591E-15	.7524E-15
-.4	-.1000E+01	.2000E+01	-.1000E+01	-.2032E-10	.3438E-15	.3307E-15
-.3	-.1000E+01	.2000E+01	-.1000E+01	-.3179E-11	.2282E-15	.2356E-15
-.2	-.1000E+01	.2000E+01	-.1000E+01	-.2334E-12	.1914E-15	.2013E-15
-.1	-.1000E+01	.2000E+01	-.1000E+01	.0000E+00	.1079E-15	.9421E-16
.0	-.1000E+01	.2000E+01	-.1000E+01	.2220E-15	.1088E-15	.1178E-15
.1	-.1000E+01	.2000E+01	-.1000E+01	-.2220E-15	.3723E-16	.4516E-16
.2	-.1000E+01	.2000E+01	-.1000E+01	-.2371E-12	.5005E-16	.3525E-16
.3	-.1000E+01	.2000E+01	-.1000E+01	-.3182E-11	.1575E-15	.1388E-15
.4	-.1000E+01	.2000E+01	-.1000E+01	-.2031E-10	.3880E-15	.3597E-15
.5	-.1000E+01	.2000E+01	-.1000E+01	-.8928E-10	.7591E-15	.7507E-15
.6	-.1000E+01	.2000E+01	-.1000E+01	-.3154E-09	.1659E-14	.1625E-14
.7	-.1000E+01	.2000E+01	-.1000E+01	-.9720E-09	.3577E-14	.3539E-14
.8	-.1000E+01	.2000E+01	-.1000E+01	-.2747E-08	.8872E-14	.8818E-14
.9	-.1000E+01	.2000E+01	-.1000E+01	-.7369E-08	.2380E-13	.2347E-13
1.0	-.1000E+01	.2000E+01	-.1000E+01	-.1926E-07	.7025E-13	.6849E-13
1.1	-.1000E+01	.2000E+01	-.1000E+01	-.5014E-07	.2325E-12	.2239E-12
1.2	-.1000E+01	.2000E+01	-.1000E+01	-.1328E-06	.8822E-12	.8363E-12
1.3	-.1000E+01	.2000E+01	-.1000E+01	-.3659E-06	.3966E-11	.3687E-11
1.4	-.1000E+01	.2001E+01	-.1000E+01	-.1078E-05	.2208E-10	.2007E-10
1.5	-.1001E+01	.2001E+01	-.1000E+01	-.3515E-05	.1629E-09	.1441E-09

Table for optimal α's and their row-sum and the square norm of local truncation error functionals, in $H^2(C_r)$-space, using Cowell's 3-points usual method and the corresponding α-optimal method, at the nodal points, with $r=2.1$, $a=-1.6$, $b=1.6$, $n=32$, $h=.1$, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; $\beta_0=1/12$, $\beta_1=10/12$, $\beta_2=1/12$.

From Table 4a, it is seen that within the tabular precision, the optimal coefficients $\hat{\alpha}_{0n}$, $\hat{\alpha}_{1n}$, $\hat{\alpha}_{2n}$ are equal to the usual coefficients α_0, α_1, α_2 and that at a general point x_n, $\|\hat{T}_n\|^2 <$ $\|T_n\|^2$, except at x = 0 and .1, where the errors are too small, so that the reversal of the inequality must be because of round-offs. Even though all the numerical calculations are performed with double precision, such small numbers might be affected by round-offs and may not be very reliable.

Table - 4b

eqn	itu	$\bar{e}_u$	ito	$\bar{e}_O$
1	2	.244871E-03	2	.128041E-03
2	2	.610703E-04	2	.192381E-04
3	3	.430195E-03	2	.286316E-03
4	2	.133292E-03	2	.544429E-04
5	2	.348263E-03	2	.555233E-03
6	3	.127772E-03	2	.879302E-04
7	2	.313175E-04	2	.202928E-04
8	2	.133523E-03	2	.538413E-04
9	2	.735570E-04	2	.214216E-04
10	1	.170782E-02	1	.141672E-02
11	1	.738872E-03	1	.276783E-03
12	1	.718937E-03	1	.260809E-03
13	2	.298705E-05	2	.220359E-05
14	2	.167071E-05	2	.102236E-05
15	2	.392662E-05	2	.327281E-05
16	2	.236517E-05	2	.185000E-05
17	1	.257920E-07	1	.170986E-07
18	1	.151826E-06	1	.331515E-07
19	3	.509406E-03	2	.285533E-03
20	3	.464907E-03	2	.257529E-03
21	2	.304135E-03	2	.264234E-04
22	2	.208304E-03	2	.192195E-04
23	2	.300455E-03	2	.637374E-03
24	2	.287372E-04	2	.487327E-04

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual and the corresponding α-optimal methods in $H^2(C_r)$-space, for 24 BVP-s.

The results in Table 4b, for BVP's with equations 1-9 and 19-24 are obtained with r=2.1, a=-1.6, b=1.6, n=32, h=.1; and the results for BVP's with equations 10-18 are obtained with r=2.8, a=-2.1, b=2.1, n=42, h=.1. It is seen from the table that the α-optimal method is producing worse results compared to the usual method for the equations 23 and 24 and this situation is not being improved with the same r and h, in the intervals [-1.8,1.8], [-1.7,1.7], [-1.5,1.5],...,[-.8,.8]. The equation 23 is giving just better result in the interval [-.7, .7], but the equation 24 still does not do so. Ultimately, in the interval [-.5, .5] both of them are giving just better results, and these results are given below.

eqn	itu	$\bar{e}_u$	ito	$\bar{e}_o$
23:	1	.445555E-05	1	.444995E-05
24:	1	.158786E-05	1	.158745E-05

The above numerical results show that as compared to the usual method the α-optimal method is one decimal place better on equations 4,6,8,18,21,22; and just better on equations 1,2,3,5,7, 9-17,19,20,23,24.

In $H^2(C_r)$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, i = $\delta_{t0}(1)k$ of β-optimal method (7) subject to the condition

$$\sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} = 1, \tag{10}$$

where α_j 's are prefixed according to some consistent and stable known usual method (8) with highest degree polynomial precision. With reference to equation (15) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where $\hat{b} = h^2\left(\hat{\beta}_{\delta_{t0},n},\ldots\ldots,\hat{\beta}_{k-1,n}\right)^T$,

$$\begin{aligned}\hat{c}_{ij} = \frac{r}{\pi}\,&\frac{2}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^3}\left[1+\frac{6x_{n+k-j}\bar{x}_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})}+\frac{6x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^2}\right]\\
&-\frac{r}{\pi}\frac{2}{(r^2-x_{n+k-j}\bar{x}_n)^3}\left[1+\frac{6x_{n+k-j}\bar{x}_n}{(r^2-x_{n+k-j}\bar{x}_n)}+\frac{6x^2_{n+k-j}\bar{x}^2_n}{(r^2-x_{n+k-j}\bar{x}_n)^2}\right]\\
&-\frac{r}{\pi}\frac{2}{(r^2-x_n\bar{x}_{n+k-i})^3}\left[1+\frac{6x_n\bar{x}_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})}+\frac{6x^2_n\bar{x}^2_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})^2}\right]\\
&+\frac{r}{\pi}\frac{2}{(r^2-x_n\bar{x}_n)^3}\left[1+\frac{6x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{6x^2_n\bar{x}^2_n}{(r^2-x_n\bar{x}_n)^2}\right],\quad i,j=\delta_{t0}(1)k-1, \text{ and}\end{aligned}$$

$$\begin{aligned}\hat{d}_i = -\frac{r}{\pi}\sum_{j=0}^{k}\alpha_j&\left\{\frac{x^2_{n+k-j}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^3}-\frac{x^2_{n+k-j}}{(r^2-x_{n+k-j}\bar{x}_n)^3}\right\}\\
&-h^2\,\frac{r}{\pi}\left[\frac{2}{(r^2-x_n\bar{x}_{n+k-i})^3}\left\{1+\frac{6x_n\bar{x}_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})}+\frac{6x^2_n\bar{x}^2_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})^2}\right\}\right.\\
&\left.-\frac{2}{(r^2-x_n\bar{x}_n)^3}\left\{1+\frac{6x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{6x^2_n\bar{x}^2_n}{(r^2-x_n\bar{x}_n)^2}\right\}\right],\qquad i=\delta_{t0}(1)k-1\end{aligned}$$

This system of equations may be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{t0}(1)k-1$.

The following theorem characterizes the β-optimal multistep method (7) in $H^2(C_r)$ space subject to the condition (10).

Theorem 5: The optimal multistep method (7) in which α_j's are prefixed and β_j's are optimized in $H^2(C_r)$ space, subject to the condition (10) is characterized by that it is locally interpolatory for functions

$$\left\{y_i(x) = \frac{x^2}{(r^2-x\bar{x}_{n+k-i})^3}-\frac{x^2}{(r^2-x\bar{x}_n)^3},\ i=\delta_{t0}(1)k-1\right\}.$$

Proof: The proof follows from Theorem 3 of Chapter 1, and the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

Table - 5a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\lVert T_n \rVert^2$	$\lVert \hat{T}_n \rVert^2$
-1.7	.6732E-03	.8838E-02	.4892E-03	.1000E-01	.1102E-05	.1568E-06
-1.6	.7375E-03	.8599E-02	.6636E-03	.1000E-01	.2478E-07	.4196E-08
-1.5	.7704E-03	.8496E-02	.7340E-03	.1000E-01	.1375E-08	.2675E-09
-1.4	.7894E-03	.8441E-02	.7692E-03	.1000E-01	.1326E-09	.2932E-10
-1.3	.8014E-03	.8409E-02	.7893E-03	.1000E-01	.1860E-10	.4671E-11
-1.2	.8095E-03	.8389E-02	.8018E-03	.1000E-01	.3431E-11	.9809E-12
-1.1	.8152E-03	.8375E-02	.8102E-03	.1000E-01	.7802E-12	.2550E-12
-1.0	.8195E-03	.8364E-02	.8161E-03	.1000E-01	.2094E-12	.7868E-13
-.9	.8227E-03	.8357E-02	.8204E-03	.1000E-01	.6440E-13	.2794E-13
-.8	.8253E-03	.8351E-02	.8237E-03	.1000E-01	.2219E-13	.1115E-13
-.7	.8273E-03	.8346E-02	.8263E-03	.1000E-01	.8485E-14	.4965E-14
-.6	.8290E-03	.8343E-02	.8284E-03	.1000E-01	.3576E-14	.2431E-14
-.5	.8304E-03	.8340E-02	.8300E-03	.1000E-01	.1626E-14	.1261E-14
-.4	.8314E-03	.8337E-02	.8313E-03	.1000E-01	.8270E-15	.7193E-15
-.3	.8323E-03	.8336E-02	.8322E-03	.1000E-01	.4759E-15	.4491E-15
-.2	.8329E-03	.8334E-02	.8328E-03	.1000E-01	.2995E-15	.2949E-15
-.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.2026E-15	.2023E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.1766E-15	.1766E-15
.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.1319E-15	.1316E-15
.2	.8328E-03	.8334E-02	.8329E-03	.1000E-01	.2288E-15	.2242E-15
.3	.8322E-03	.8336E-02	.8323E-03	.1000E-01	.4405E-15	.4138E-15
.4	.8313E-03	.8337E-02	.8314E-03	.1000E-01	.8094E-15	.7017E-15
.5	.8300E-03	.8340E-02	.8304E-03	.1000E-01	.1608E-14	.1243E-14
.6	.8284E-03	.8343E-02	.8290E-03	.1000E-01	.3523E-14	.2378E-14
.7	.8263E-03	.8346E-02	.8273E-03	.1000E-01	.8555E-14	.5036E-14
.8	.8237E-03	.8351E-02	.8253E-03	.1000E-01	.2230E-13	.1126E-13
.9	.8204E-03	.8357E-02	.8227E-03	.1000E-01	.6440E-13	.2794E-13
1.0	.8161E-03	.8364E-02	.8195E-03	.1000E-01	.2094E-12	.7862E-13
1.1	.8102E-03	.8375E-02	.8152E-03	.1000E-01	.7802E-12	.2550E-12
1.2	.8018E-03	.8389E-02	.8095E-03	.1000E-01	.3431E-11	.9809E-12
1.3	.7893E-03	.8409E-02	.8014E-03	.1000E-01	.1860E-10	.4672E-11
1.4	.7692E-03	.8441E-02	.7894E-03	.1000E-01	.1326E-09	.2932E-10
1.5	.7340E-03	.8496E-02	.7704E-03	.1000E-01	.1375E-08	.2675E-09
1.6	.6636E-03	.8599E-02	.7375E-03	.1000E-01	.2478E-07	.4196E-08
1.7	.4892E-03	.8838E-02	.6732E-03	.1000E-01	.1102E-05	.1568E-06

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using 3-points Cowell's usual method and the corresponding β-optimal method with restriction, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1, α_0=-1, α_1=2; α_2=-1; β_0=1/12, β_1=10/12, β_2=1/12, in $H^2(C_r)$ space.

Table 5a shows that the optimal coefficients $\hat{\beta}_{0n}$, $\hat{\beta}_{1n}$, $\hat{\beta}_{2n}$ are changing from point to point and at a general point x_n, $\lVert \hat{T}_n \rVert^2 \le$

$\|T_n\|^2$. In a neighbourhood of x=0, $\hat{\beta}_{in}$'s are very close to the usual coefficients β_i's and $\|\hat{T}_n\|^2$, $\|T_n\|^2$ are numerically equal.

Table - 5b

eqn	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.682802E-04
2	2	.610703E-04	2	.281577E-04
3	3	.430195E-03	2	.104135E-03
4	2	.133292E-03	2	.362855E-04
5	2	.348263E-03	2	.135079E-03
6	3	.127772E-03	2	.338500E-04
7	2	.313175E-04	2	.835447E-05
8	2	.133523E-03	2	.376090E-04
9	2	.735570E-04	2	.207658E-04
10	1	.170782E-02	1	.309772E-03
11	1	.738872E-03	1	.706424E-04
12	1	.718937E-03	1	.609621E-04
13	2	.298705E-05	2	.114488E-05
14	2	.167071E-05	2	.625330E-06
15	2	.392662E-05	2	.149686E-05
16	2	.236517E-05	2	.833412E-06
17	1	.257920E-07	1	.928588E-08
18	1	.151826E-06	1	.553283E-07
19	3	.509406E-03	2	.132122E-03
20	3	.464907E-03	2	.122836E-03
21	2	.304135E-03	2	.917673E-04
22	2	.208304E-03	2	.627561E-04
23	2	.300455E-03	2	.104856E-03
24	2	.287372E-04	2	.121353E-04

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual and the corresponding β-optimal methods with restriction, in $H^2(C_r)$-space, for 24 BVP-s.

The numerical results in Table 5b, on 24 BVP-s for equations 1-9 and 19-24 are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1; and for equations 10-18, with r=2.8, a=-2.1, b=2.1, n=42, h=.1. As compared to usual method, β-optimal method with restriction for BVP is one decimal place better on equations 1,4,6-8,10-12,14,16 - 18, 21,22; and just better on equations 2,3,5,9,13,15,19,20,23 and 24.

Table - 5c

eqn	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.410628E-02
2	4	.250457E-02	4	.101724E-02
3	8	.760039E-01	5	.167955E-01
4	5	.132805E-01	4	.338135E-02
5	4	.716823E-02	4	.290794E-02
6	5	.356402E-02	4	.100650E-02
7	4	.354625E-03	3	.103725E-03
8	4	.211573E-02	4	.639029E-03
9	3	.604542E-03	3	.187586E-03
10	4	.119641E-01	4	.621026E-02
11	4	.130464E+00	4	.193414E-01
12	4	.129361E+00	4	.189977E-01
13	2	.128426E-05	2	.561091E-06
14	2	.831124E-06	1	.347910E-06
15	2	.193794E-05	2	.877730E-06
16	2	.130401E-05	2	.563117E-06
17	1	.456442E-08	1	.814943E-09
18	1	.343343E-07	1	.226087E-08
19	11	.103867E+00	6	.208003E-01
20	4	.188589E-02	3	.499274E-03
21	4	.112364E-02	3	.326909E-03
22	5	.115497E-01	4	.332103E-02
23	4	.610397E-02	4	.235365E-02
24	3	.542588E-04	2	.733719E-05

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual and the corresponding β-optimal methods with restriction, in $H^2(C_r)$-space, for 24 IVP-s.

The numerical results of Table 5b on 24 IVP-s, are obtained for equations 1-9 and 19-24, with r=2.01, a=-1.7, b=1.7, n=34, h=.1; and for equations 10-18, with r=2.7, a=-1.4, b=1.4, n=28, h=.1. As compared to usual method, β-optimal method with restriction for IVP is one decimal place better on equations 1,4,8,10-13,15-22 and 24; and just better on equations 2,3,5,6,7,9, 14 and 23.

In $H^2(C_r)$ space, we have to determine the optimal coefficients

$\hat{\alpha}_{i,n}, i = 0(1)k$ and $\hat{\beta}_{i,n}, i = \delta_{t0}(1)k-1$ of an (α,β)-optimal multistep method

(11) $$\sum_{j=0}^{k} \hat{\alpha}_{j,n} y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} f_{n+k-j} = 0,$$

subject to the condition (10). With reference to equation (18) and (19) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d}, \quad \text{where}$$

$$\hat{b} = \left(\hat{\alpha}_{0,n}, \ldots\ldots, \hat{\alpha}_{k,n}, h^2\hat{\beta}_{\delta_{t0},n}, \ldots\ldots, h^2\hat{\beta}_{k-1,n} \right)^T;$$

$$\hat{C}_{ij} = \frac{r}{2\pi(r^2 - x_{n+k-j}\bar{x}_{n+k-i})}, \quad i, j = 0(1)k;$$

$$\hat{C}_{ij} = \frac{r\bar{x}^2_{n+k-i}}{\pi(r^2 - \bar{x}_{n+k-i}x_{n+k-j})^3} - \frac{r\bar{x}^2_{n+k-i}}{\pi(r^2 - \bar{x}_{n+k-i}x_n)^3}, \quad i = 0(1)k, \quad j = k+1(1)2k+1-\delta_{t0};$$

$$\hat{C}_{ij} = \frac{rx^2_{n+k-j}}{\pi(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^3} - \frac{rx^2_{n+k-j}}{\pi(r^2 - x_{n+k-j}\bar{x}_n)^3}, \quad i = k+1(1)2k+1-\delta_{t0}, \quad j = 0(1)k;$$

$$\hat{C}_{ij} = \frac{r}{\pi}\frac{2}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^3}\left[1+\frac{6x_{n+k-j}\bar{x}_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})}+\frac{6x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^2}\right]$$

$$-\frac{r}{\pi}\frac{2}{(r^2-x_{n+k-j}\bar{x}_n)^3}\left[1+\frac{6x_{n+k-j}\bar{x}_n}{(r^2-x_{n+k-j}\bar{x}_n)}+\frac{6x^2_{n+k-j}\bar{x}^2_n}{(r^2-x_{n+k-j}\bar{x}_n)^2}\right]$$

$$-\frac{r}{\pi}\frac{2}{(r^2-x_n\bar{x}_{n+k-i})^3}\left[1+\frac{6x_n\bar{x}_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})}+\frac{6x^2_n\bar{x}^2_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})^2}\right]$$

$$+\frac{r}{\pi}\frac{2}{(r^2-x_n\bar{x}_n)^3}\left[1+\frac{6x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{6x^2_n\bar{x}^2_n}{(r^2-x_n\bar{x}_n)^2}\right], \quad \text{for } i,j=k+1(1)2k+1-\delta_{t0};$$

$$\hat{d}_i = h^2 \frac{r\bar{x}^2_{n+k-1}}{\pi(r^2 - \bar{x}_{n+k-1}x_n)^3}, \qquad i = 0(1)k;$$

$$\hat{d}_i = -\frac{r}{\pi} h^2 \Bigg[\frac{2}{(r^2-x_n\bar{x}_{n+k-1})^3}\left\{1+\frac{6x_n\bar{x}_{n+k-1}}{(r^2-x_n\bar{x}_{n+k-1})}+\frac{6x_n^2\bar{x}^2_{n+k-1}}{(r^2-x_n\bar{x}_{n+k-1})^2}\right\}$$

$$-\frac{2}{(r^2-x_n\bar{x}_n)^3}\left\{1+\frac{6x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{6x_n^2\bar{x}_n^2}{(r^2-x_n\bar{x}_n)^2}\right\}\Bigg], \quad \text{for } i=k+1(1)2k+1-\delta_{t0}.$$

The following theorem characterizes the (α,β)-optimal method (11) in $H^2(C_r)$ space subject to the condition (10).

Theorem 6: The optimal multistep method (11) in which α_j's as well as β_j's are optimized in $H^2(C_r)$ space, subject to the condition (10) is characterized by that it is locally interpolatory for functions $\{y_{1i}(x),\ i = \delta_{t0}(1)k-1\} \cup \{y_{2i}(x),\ i = 0(1)k-1\}$,

where $$y_{1i}(x) = \frac{x^2}{(r^2-x\bar{x}_{n+k-i})^3} - \frac{x^2}{(r^2-x\bar{x}_n)^3}, \quad i = \delta_{t0}(1)k-1$$

and $$y_{2i}(x) = \frac{1}{(r^2-x\bar{x}_{n+k-i})}, \quad i = 0(1)k-1.$$

Proof: The proof follows from Theorem 4 of Chapter 1, and the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

4.4 Optimal Multistep Methods in $H^2(C_r)$-Space Interpolatory for Polynomials.

In Chapter 1, we have given an approach for determining the optimal multistep methods interpolatory for polynomials of certain degree, in a general Hilbert space with reproducing kernel function. We know

$$(12) \qquad \sum_{j=0}^{k}\alpha_j y_{n+k-j} + h^2\sum_{j=0}^{k-\delta_{t0}}\gamma_j \nabla^j f(x_{n+k-\delta_{t0}}, y_{n+k-\delta_{t0}}) = 0$$

represents a general k-step method for a second order differential equation. A general method interpolatory for polynomials of degree $q < k+\delta_{t1}+1$, can be written as

$$(13) \qquad \sum_{j=0}^{k}\alpha_j y_{n+k-j} + h^2\sum_{j=0}^{q-2}\gamma_j^u \nabla^j f(x_{n+k-\delta_{t0}}, y_{n+k-\delta_{t0}}) =$$

$$- h^2\sum_{j=q-1}^{k-\delta_{t0}}\gamma_j \nabla^j f(x_{n+k-\delta_{t0}}, y_{n+k-\delta_{t0}}),$$

with prefixed α_j's such that $\sum_{j=0}^{k}\alpha_j = 0$ and $\sum_{j=0}^{k} j\alpha_j = 0$, where α_j's and γ_j^u 's are according to the corresponding usual method. The remaining coefficients, γ_j, $j = q-1(1)k-\delta_{t0}$, can be determined by minimizing the norm of the local truncation error functional of the method over the Hilbert space $H^2(C_r)$. Let us denote the optimized coefficients as $\hat{\gamma}_{j,n}$, $j = q-1(1)k-\delta_{t0}$.

The local truncation error for the optimal method (13) is

$$\sum_{j=0}^{k}\alpha_j y(x_{n+k-j}) + h^2\sum_{j=0}^{q-2}\gamma_j^u \nabla^j y''(x_{n+k-\delta_{t0}})$$

$$+ h^2\sum_{j=q-1}^{k-\delta_{t0}}\hat{\gamma}_{j,n} \nabla^j y''(x_{n+k-\delta_{t0}}).$$

Since, $\nabla^j y''(x_{n+k-\delta_{t0}}) = \sum_{i=0}^{j}(-1)^i\, {}^jC_i\, y''(x_{n+k-\delta_{t0}-i})$, the representer for $\nabla^j y''(x_{n+k-\delta_{t0}})$ in $H^2(C_r)$ space is $\sum_{i=0}^{j}(-1)^i\, {}^jC_i\, D2(t,\bar{x}_{n+k-\delta_{t0}-i})$. The representer for the local truncation error functional of the optimal method in $H^2(C_r)$-space is then given by

$$\hat{T}_n^q = \sum_{j=0}^{k} \bar{\alpha}_j K(t,\bar{x}_{n+k-j}) + h^2 \sum_{j=0}^{q-2} \bar{\gamma}_j^u \sum_{i=0}^{j} (-1)^i \, {}^jC_i D2(t,\bar{x}_{n+k-\delta_{t0}-i})$$

$$+ h^2 \sum_{j=q-1}^{k-\delta_{t0}} \bar{\hat{\gamma}}_{j,n} \sum_{i=0}^{j} (-1)^i \, {}^jC_i D2(t,\bar{x}_{n+k-\delta_{t0}-i}).$$

Since $\{K(t,\bar{x}_{n+k-i}),\ i = 0(1)k;\ D2(t,\bar{x}_{n+k-i}),\ i = 0(1)k\}$ is linearly independent, to minimize $\| \hat{T}_n^q \|$ with respect to $\hat{\gamma}_{l,n}$, $\delta(\|\hat{T}_n^q\|)$ following a change $\delta(\hat{\gamma}_{l,n})$ in $\hat{\gamma}_{l,n}$, $l = q-1(1)k-\delta_{t0}$, is to vanish. Proceeding as earlier we get the following system of normal equations:

$$\sum_{l=0}^{i} (-1)^l \, {}^iC_l \left[D2(t,\bar{x}_{n+k-\delta_{t0}-l}), \sum_{j=0}^{k} \bar{\alpha}_j K(t,\bar{x}_{n+k-j})\right]$$

$$+h^2 \sum_{l=0}^{i} (-1)^l \, {}^iC_l \left[D2(t,\bar{x}_{n+k-\delta_{t0}-l}), \sum_{j=0}^{q-2} \bar{\gamma}_j^u \sum_{m=0}^{j} (-1)^m \, {}^jC_m D2(t,\bar{x}_{n+k-\delta_{t0}-m})\right]$$

$$+h^2 \sum_{l=0}^{i} (-1)^l \, {}^iC_l \Bigg[D2(t,\bar{x}_{n+k-\delta_{t0}-l}),$$

$$\sum_{j=q-1}^{k-\delta_{t0}} \bar{\hat{\gamma}}_{j,n} \sum_{m=0}^{j} (-1)^m \, {}^jC_m D2(t,\bar{x}_{n+k-\delta_{t0}-m})\Bigg] = 0, \quad i = q-1(1)k-\delta_{t0},$$

$$\text{or,} \quad \sum_{j=0}^{k} \alpha_j \sum_{l=0}^{i} (-1)^l \, {}^iC_l \ D2(x_{n+k-j},\bar{x}_{n+k-\delta_{t0}-l})$$

$$+h^2 \sum_{j=0}^{q-2} \gamma_j^u \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m} \, {}^iC_l \, {}^jC_m D2''(x_{n+k-\delta_{t0}-m},\bar{x}_{n+k-\delta_{t0}-l})$$

$$+h^2 \sum_{j=q-1}^{k-\delta_{t0}} \hat{\gamma}_{j,n} \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m} \, {}^iC_l \, {}^jC_m D2''(x_{n+k-\delta_{t0}-m},\bar{x}_{n+k-\delta_{t0}-l}) = 0,$$

$$\text{for} \quad i = q-1(1)k-\delta_{t0},$$

or, $$\hat{C}\,\hat{b} = \hat{d},$$

where $\hat{b} = \left(\hat{\gamma}_{q-1,n}, \hat{\gamma}_{q,n}, \ldots\ldots, \hat{\gamma}_{k-\delta_{t0},n}\right)^T$,

$$\hat{C}_{ij} = h^2 \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\, {}^iC_l\, {}^jC_m\, \frac{r}{\pi}\, \frac{2}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})^3} \cdot$$

$$\left[1 + \frac{6x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l}}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})} + \frac{6x^2_{n+k-\delta_{t0}-m}\bar{x}^2_{n+k-\delta_{t0}-l}}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})^2}\right],$$

$$\hat{d}_i = -\sum_{j=0}^{k} \alpha_j \sum_{l=0}^{i} (-1)^l\, {}^iC_l\, \frac{r x^2_{n+k-j}}{\pi(r^2 - x_{n+k-j}\bar{x}_{n+k-\delta_{t0}-l})^3}$$

$$- h^2 \sum_{j=0}^{q-2} \gamma_j^u \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\, {}^iC_l\, {}^jC_m \frac{r}{\pi}\, \frac{2}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})^3} \cdot$$

$$\cdot\left[1 + \frac{6x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l}}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})} + \frac{6x^2_{n+k-\delta_{t0}-m}\bar{x}^2_{n+k-\delta_{t0}-l}}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})^2}\right],$$

for $i = q-1(1)k-\delta_{t0}$.

Thus we get the following theorem.

<u>Theorem 7</u>: The optimal multistep method (13) interpolatory for polynomials of degree q is characterized by that it is locally interpolatory for functions

$$\{x^i;\ i = 1(1)q\} \cup \{h_i(x);\ i = q-1(1)k-\delta_{t0}\},$$

where $h_i(x) = \sum_{l=0}^{i} (-1)^l\, {}^iC_l\, \dfrac{x^2}{(r^2 - x\bar{x}_{n+k-\delta_{t0}-l})^3}$.

We next discuss an α-optimal multistep method interpolatory for polynomials of degree q, in $H^2(C_r)$-space, in terms of backward differences

(14) $$\sum_{j=2}^{k} \gamma_j \nabla^j y_{n+k} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0,$$

represents a general k-step method for a 2-nd order differential equation. A general method interpolatory for polynomials of degree q can be written as

(15) $$\sum_{j=2}^{q} \gamma_j^u \nabla^j y_{n+k} + \sum_{j=q+1}^{k} \gamma_j \nabla^j y_{n+k} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0,$$

where the coefficients γ_j^u 's are defined as in the corresponding usual method. The remaining coefficients γ_j, j = q+1(1)k can be determined by minimizing the norm of the local truncation error functional of the method over the Hilbert space $H^2(C_r)$. Let us denote the optimized coefficients as $\hat{\gamma}_{j,n}$, j = q+1(1)k.

The representer for the local truncation error functional for the optimal method (15) is given by

$$\hat{T}_n^q = \sum_{j=2}^{q} \bar{\gamma}_j^u \sum_{l=0}^{j} (-1)^l \; {}^jC_l K(t,\bar{x}_{n+k-l})$$
$$+ \sum_{j=q+1}^{k} \bar{\hat{\gamma}}_{j,n} \sum_{l=0}^{j} (-1)^l \; {}^jC_l K(t,\bar{x}_{n+k-l}) + h^2 \sum_{j=\delta_{t0}}^{k} \bar{\beta}_j D2(t,\bar{x}_{n+k-j}).$$

Since S = $\{K(t,\bar{x}_{n+k-j})$, j=0(1)k; $D2(t,\bar{x}_{n+k-j})$, j=0(1)k$\}$ is linearly independent, to minimize $\| \hat{T}_n^q \|$ with respect to $\hat{\gamma}_{l,n}$, $\delta(\|\hat{T}_n^q\|)$, following a change $\delta(\hat{\gamma}_{l,n})$ in $\hat{\gamma}_{l,n}$, l = q+1(1)k, is to vanish. Proceeding as earlier we get the following normal equations.

$$\sum_{j=2}^{q}\gamma_j^u \sum_{m=0}^{j}\sum_{l=0}^{i}(-1)^{l+m}\ {}^iC_l\ {}^jC_m\ K(x_{n+k-m}\ ,\ \bar{x}_{n+k-l})$$

$$+\sum_{j=q+1}^{k}\hat{\gamma}_{j,n}\sum_{m=0}^{j}\sum_{l=0}^{i}(-1)^{l+m}\ {}^iC_l\ {}^jC_m\ K(x_{n+k-m}\ ,\ \bar{x}_{n+k-l})$$

$$+\ h^2\sum_{j=\delta_{t0}}^{k}\beta_j\sum_{l=0}^{i}(-1)^l\ {}^iC_l\ \overline{D2(x_{n+k-l}\ ,\ \bar{x}_{n+k-j})} = 0, \quad i = q+1(1)k,$$

or, $\hat{C}\ \hat{a} = \hat{d}$, where

$$\hat{a} = \left(\hat{\gamma}_{q+1,n},\ldots\ldots,\hat{\gamma}_{k,n}\right)^T,$$

$$\hat{c}_{ij} = \sum_{m=0}^{j}\sum_{l=0}^{i}(-1)^{l+m}\ {}^iC_l\ {}^jC_m\frac{r}{2\pi(r^2-x_{n+k-m}\bar{x}_{n+k-l})}, \quad i,j = q+1(1)k,$$

$$\hat{d}_i = -\sum_{j=2}^{q}\gamma_j^u\sum_{m=0}^{j}\sum_{l=0}^{i}(-1)^{l+m}\ {}^iC_l\ {}^jC_m\frac{r}{2\pi(r^2-x_{n+k-m}\bar{x}_{n+k-l})}$$

$$-\ h^2\sum_{j=\delta_{t0}}^{k}\beta_j\sum_{l=0}^{i}(-1)^l\ {}^iC_l\frac{r\bar{x}^2_{n+k-l}}{\pi(r^2-\bar{x}_{n+k-l}x_{n+k-j})^3}, \quad i = q+1(1)k.$$

Hence we get the following:

<u>Theorem 8</u> : The optimal multistep method (15) interpolatory for polynomials of degree q is characterized by that it is locally interpolatory for functions

$$\{x^i;\ i = 1(1)q\} \cup \{h_i(x);\ i = q+1(1)k\},$$

where $h_i(x) = \sum_{l=0}^{i}(-1)^l\ {}^iC_l\ \dfrac{1}{(r^2-x\bar{x}_{n+k-l})}, \quad i = q+1(1)k.$

We implemented β-optimal method interpolatory for polynomials of degree 2, and the numerical results turn out to be the same as those of β-optimal method with restriction (10), as is to be expected theoretically also. The two procedures in this case thus becoming only alternate implementations of theoretically the same formulae. Hence we are presenting the numerical results for β-optimal method interpolatory for polynomials of degree 3 which constrains more than the requirement (10).

From Table 6a, it is seen that the optimal $\hat{\beta}_{in}$'s are depending on the nodal points and in a neighborhood of the origin the optimal $\hat{\beta}_{in}$'s are close to the corresponding usual β_i's. At a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$, however in a neighborhood of x=0, $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are almost equal. We also note that $\hat{\beta}_{0n} = \hat{\beta}_{2n}$, and that $\hat{\beta}_{0n}+\hat{\beta}_{1n}+\hat{\beta}_{2n} = 1$, which can be shown to be true on theoretical grounds also.

In Table 6b, the numerical results for BVP's with equations 1-9 and 19-24 are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1; and the results for BVP's with equations 10-18 are obtained with r=2.8, a=-2.1, b=2.1, n=42, h=.1. Table 5b reveals that as compared to usual method, β-optimal method interpolatory for polynomials of degree 3 for BVP is two decimal places better on equation 18; one decimal place better on equations 1,3-10,13,14,16,17,20-24; and just better on equations 2,11,12 ,15,19.

Table - 6a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\Vert T_n\Vert^2$	$\Vert\hat{T}_n\Vert^2$
-1.7	.7339E-03	.8532E-02	.7339E-03	.1000E-01	.1102E-05	.3392E-06
-1.6	.7785E-03	.8443E-02	.7785E-03	.1000E-01	.2478E-07	.8666E-08
-1.5	.7988E-03	.8402E-02	.7988E-03	.1000E-01	.1375E-08	.5247E-09
-1.4	.8098E-03	.8380E-02	.8098E-03	.1000E-01	.1326E-09	.5445E-10
-1.3	.8164E-03	.8367E-02	.8164E-03	.1000E-01	.1860E-10	.8190E-11
-1.2	.8207E-03	.8359E-02	.8207E-03	.1000E-01	.3431E-11	.1618E-11
-1.1	.8237E-03	.8353E-02	.8237E-03	.1000E-01	.7802E-12	.3948E-12
-1.0	.8258E-03	.8348E-02	.8258E-03	.1000E-01	.2094E-12	.1140E-12
-.9	.8274E-03	.8345E-02	.8274E-03	.1000E-01	.6440E-13	.3781E-13
-.8	.8287E-03	.8343E-02	.8287E-03	.1000E-01	.2219E-13	.1410E-13
-.7	.8297E-03	.8341E-02	.8297E-03	.1000E-01	.8485E-14	.5866E-14
-.6	.8305E-03	.8339E-02	.8305E-03	.1000E-01	.3576E-14	.2701E-14
-.5	.8312E-03	.8338E-02	.8312E-03	.1000E-01	.1626E-14	.1335E-14
-.4	.8319E-03	.8336E-02	.8319E-03	.1000E-01	.8270E-15	.7366E-15
-.3	.8324E-03	.8335E-02	.8324E-03	.1000E-01	.4759E-15	.4520E-15
-.2	.8329E-03	.8334E-02	.8329E-03	.1000E-01	.2995E-15	.2951E-15
-.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.2026E-15	.2023E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.1766E-15	.1766E-15
.1	.8332E-03	.8334E-02	.8332E-03	.1000E-01	.1319E-15	.1316E-15
.2	.8329E-03	.8334E-02	.8329E-03	.1000E-01	.2288E-15	.2244E-15
.3	.8324E-03	.8335E-02	.8324E-03	.1000E-01	.4405E-15	.4166E-15
.4	.8319E-03	.8336E-02	.8319E-03	.1000E-01	.8094E-15	.7190E-15
.5	.8312E-03	.8338E-02	.8312E-03	.1000E-01	.1608E-14	.1318E-14
.6	.8305E-03	.8339E-02	.8305E-03	.1000E-01	.3523E-14	.2648E-14
.7	.8297E-03	.8341E-02	.8297E-03	.1000E-01	.8555E-14	.5937E-14
.8	.8287E-03	.8343E-02	.8287E-03	.1000E-01	.2230E-13	.1420E-13
.9	.8274E-03	.8345E-02	.8274E-03	.1000E-01	.6440E-13	.3781E-13
1.0	.8258E-03	.8348E-02	.8258E-03	.1000E-01	.2094E-12	.1139E-12
1.1	.8237E-03	.8353E-02	.8237E-03	.1000E-01	.7802E-12	.3947E-12
1.2	.8207E-03	.8359E-02	.8207E-03	.1000E-01	.3431E-11	.1618E-11
1.3	.8164E-03	.8367E-02	.8164E-03	.1000E-01	.1860E-10	.8190E-11
1.4	.8098E-03	.8380E-02	.8098E-03	.1000E-01	.1326E-09	.5445E-10
1.5	.7988E-03	.8402E-02	.7988E-03	.1000E-01	.1375E-08	.5247E-09
1.6	.7785E-03	.8443E-02	.7785E-03	.1000E-01	.2478E-07	.8666E-08
1.7	.7339E-03	.8532E-02	.7339E-03	.1000E-01	.1102E-05	.3392E-06

Table for optimal β's, their row-sum and the square norm of local truncation error functionals for Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; α_0=-1, α_1=2, α_2=-1; β_0=.083333, β_1=.833333, β_2=.083333; γ_0=1, γ_1=-1, γ_2=1/12, in $H^2(C_r)$ space.

Table - 6b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.237657E-04
2	2	.610703E-04	2	.269937E-04
3	3	.430195E-03	2	.664668E-04
4	2	.133292E-03	2	.290150E-04
5	2	.348263E-03	2	.364906E-04
6	3	.127772E-03	2	.310152E-04
7	2	.313175E-04	2	.758292E-05
8	2	.133523E-03	2	.135525E-04
9	2	.735570E-04	2	.758457E-05
10	1	.170782E-02	1	.462419E-03
11	1	.738872E-03	1	.657043E-03
12	1	.718937E-03	1	.653502E-03
13	2	.298705E-05	2	.846255E-06
14	2	.167071E-05	1	.220927E-06
15	2	.392662E-05	2	.147731E-05
16	2	.236517E-05	2	.643198E-06
17	1	.257920E-07	1	.646324E-08
18	1	.151826E-06	1	.374333E-08
19	3	.509406E-03	2	.104757E-03
20	3	.464907E-03	2	.949003E-04
21	2	.304134E-03	2	.185829E-04
22	2	.208304E-03	2	.117549E-04
23	2	.300455E-03	2	.552848E-04
24	2	.287372E-04	2	.434804E-05

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual method and the corresponding β-optimal method in $H^2(C_r)$ space, interpolatory for polynomials of degree 3, for 24 BVP-s.

The results in Table 6c for IVP's with equations 1-9 and 19-24 are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1; and the results for IVP's with equations 10 - 18 are obtained with r=2.7, a=-1.4, b=1.4, n=28, h=.1. Table 6c reveals that as compared to usual method, β-optimal method interpolatory for polynomials of degree 3 for IVP is two decimal places better on equations 21,22; one decimal place better on equations 1,2,4-20,23,24; and just better on equation 3.

Table - 6c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.159452E-02
2	4	.250457E-02	3	.814122E-03
3	8	.760039E-01	5	.119945E-01
4	5	.132805E-01	4	.141468E-02
5	4	.716823E-02	3	.617527E-03
6	5	.356402E-02	4	.924177E-03
7	4	.354625E-03	3	.935203E-04
8	4	.211573E-02	3	.258687E-03
9	3	.604542E-03	3	.763205E-04
10	4	.119641E-01	4	.738774E-02
11	4	.130464E+00	4	.191610E-01
12	4	.129361E+00	4	.184267E-01
13	2	.128426E-05	2	.370888E-06
14	2	.831124E-06	1	.169616E-06
15	2	.193794E-05	2	.750076E-06
16	2	.130401E-05	2	.429099E-06
17	1	.456442E-08	1	.708386E-09
18	1	.343343E-07	1	.249902E-08
19	11	.103867E+00	6	.179523E-01
20	4	.188589E-02	3	.433292E-03
21	4	.112364E-02	3	.978492E-04
22	5	.115497E-01	4	.884308E-03
23	4	.610397E-02	3	.901793E-03
24	3	.542588E-04	2	.622506E-05

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual method and the corresponding β-optimal method in $H^2(C_r)$ space, interpolatory for polynomials of degree 3, for 24 IVP-s.

4.5 <u>Optimal Multistep Methods in $H^2(C_r)$-Space Interpolatory for A Set of Pre assigned Functions.</u>

To obtain the coefficients $\hat{\beta}^F_{j,n}$, $j = \delta_{t0}(1)k$ of a β-optimal multistep method

$$\sum_{j=0}^{k} \alpha_j \, y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,n} \, f_{n+k-j} = 0, \tag{16}$$

in $H^2(C_r)$ space with prefixed α_j's, interpolatory for q number of

linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$; we have to solve a system of linear equations given in the matrix form as

$$\begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix}\begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where $A = (A_{ij})_{\substack{i=\delta_{t0}(1)k, \\ j=\delta_{t0}(1)k}}$ with

$$A_{ij} = \frac{r}{\pi}\,\frac{2}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^3}\left[1 + \frac{6x_{n+k-j}\bar{x}_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})} + \frac{6x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}\right],$$

$F = (F_{ij})_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k}}$, with $F_{ij} = f''_i\,(x_{n+k-j})$,

$b = h^2\left(\hat{\beta}^F_{\delta_{t0},n}, \hat{\beta}^F_{\delta_{t0}+1,n}, \ldots, \hat{\beta}^F_{k,n}\right)^T$, $\lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q)^T$,

$c = \left(c_{\delta_{t0}}, c_{\delta_{t0}+1}, \ldots, c_k\right)^T$, with $c_i = -\sum_{j=0}^{k} \alpha_j \frac{r}{\pi}\frac{x^2_{n+k-j}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^3}$,

$f = [\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q]^T$, with $\tilde{f}_i = -\sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j})$.

This method is characterized as follows:

Theorem 9: The β-optimal multistep method (16), in $H^2(C_r)$ space, interpolatory for linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$; is characterized by that it is locally interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i(x);\ i = \delta_{t0}(1)k-q\},$$

where $h_i(x) = \dfrac{x^2}{(r^2 - x\bar{x}_{n+k-i})^3} - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\,i+1-\delta_{t0}} \dfrac{x^2}{(r^2 - x\bar{x}_{n+k-j})^3}$

and $G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}}$, where

$$P = \left(f_i'' \; (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=k-q+1(1)k}} \quad \text{and} \quad E = \left(f_i'' \; (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-q}} .$$

Proof: The proof follows from Theorem 8 of Chapter 1.

To obtain the coefficients $\hat{\alpha}^F_{j,n}$, $j = 0(1)k$ of an α-optimal multistep method

(17) $$\sum_{j=0}^{k} \hat{\alpha}^F_{j,n} \, y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \, f_{n+k-j} = 0,$$

in $H^2(C_r)$ space with prefixed β_j's, interpolatory for q number of linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$; we have to solve a system of linear equations given in the matrix form as

$$\begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} a \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where $A = (A_{ij})_{\substack{i=0(1)k \\ j=0(1)k}}$; with $A_{ij} = \dfrac{r}{2\pi} \dfrac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})}$,

$F = (F_{ij})_{\substack{i=1(1)q \\ j=0(1)k}}$; with $F_{ij} = f_i(x_{n+k-j})$,

$$a = \left(\hat{\alpha}^F_{0,n}, \hat{\alpha}^F_{1,n}, \ldots, \hat{\alpha}^F_{k,n}\right)^T, \qquad \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q)^T,$$

$c = (c_0, c_1, \ldots, c_k)^T$; with $c_i = -h^2 \displaystyle\sum_{j=\delta_{t0}}^{k} \beta_j \frac{r}{\pi} \frac{x^2_{n+k-i}}{(r^2 - x_{n+k-i}\bar{x}_{n+k-j})^3}$,

$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T$; with $\tilde{f}_i = -h^2 \displaystyle\sum_{j=\delta_{t0}}^{k} \beta_j f_i''(x_{n+k-j})$.

This method is characterized as follows.

<u>Theorem 10</u>: An α-optimal multistep method (10), in $H^2(C_r)$ space interpolatory for arbitrary functions $f_1, f_2, \ldots, f_q$ is characterized by that it is locally interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i(x);\ i = 0(1)k-q\},$$

where $h_i(x) = \dfrac{1}{(r^2 - x\bar{x}_{n+k-i})} - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1} \dfrac{1}{(r^2 - x\bar{x}_{n+k-j})}$,

and $G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}}$, where

$$P = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=k-q+1(1)k}} \quad \text{and} \quad E = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=0(1)k-q}} .$$

<u>Proof</u>: The proof follows from the Theorem 9 of Chapter 1.

In the following tables we are presenting the numerical results of β-optimal method interpolatory for linearly independent functions exp(1.6x) and exp(-1.6x).

Table 7a reveals that the optimal $\hat{\beta}_{in}$'s are depending on nodal points and in a neighborhood of the origin the optimal $\hat{\beta}_{in}$'s are close to the corresponding usual β_i's. At a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$ but at x=-.1,0,.1; this inequality does not hold in the numerical values. This must be because of round-offs of order $O(10^{-17})$.

The numerical results of Table 7b for BVP's with equations 1-9 and 19-24 are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1; and the results for BVP's with equations 10-18 are obtained with r=2.8, a=-2.1, b=2.1, n=42, h=.1. Table 7b reveals that as compared to usual method β-optimal method interpolatory for linearly independent functions exp (1.6x) and exp (-1.6x) for BVP's is one

decimal place better on equations 1,3-10, 14,16-18,20-24; and just better on equations 2,11-13,15 and 19.

Table - 7a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\lVert T_n \rVert^2$	$\lVert \hat{T}_n \rVert^2$
-1.7	.7321E-03	.8538E-02	.7321E-03	.1000E-01	.1102E-05	.3305E-06
-1.6	.7765E-03	.8448E-02	.7765E-03	.1000E-01	.2478E-07	.8311E-08
-1.5	.7969E-03	.8407E-02	.7969E-03	.1000E-01	.1375E-08	.4946E-09
-1.4	.8079E-03	.8385E-02	.8079E-03	.1000E-01	.1326E-09	.5047E-10
-1.3	.8147E-03	.8371E-02	.8147E-03	.1000E-01	.1860E-10	.7485E-11
-1.2	.8191E-03	.8362E-02	.8191E-03	.1000E-01	.3431E-11	.1466E-11
-1.1	.8222E-03	.8356E-02	.8222E-03	.1000E-01	.7802E-12	.3572E-12
-1.0	.8246E-03	.8351E-02	.8246E-03	.1000E-01	.2094E-12	.1039E-12
-.9	.8265E-03	.8347E-02	.8265E-03	.1000E-01	.6440E-13	.3503E-13
-.8	.8280E-03	.8344E-02	.8280E-03	.1000E-01	.2219E-13	.1335E-13
-.7	.8293E-03	.8342E-02	.8293E-03	.1000E-01	.8485E-14	.5682E-14
-.6	.8304E-03	.8339E-02	.8304E-03	.1000E-01	.3576E-14	.2663E-14
-.5	.8312E-03	.8338E-02	.8312E-03	.1000E-01	.1626E-14	.1329E-14
-.4	.8319E-03	.8336E-02	.8319E-03	.1000E-01	.8270E-15	.7351E-15
-.3	.8323E-03	.8335E-02	.8323E-03	.1000E-01	.4759E-15	.4525E-15
-.2	.8326E-03	.8335E-02	.8326E-03	.1000E-01	.2995E-15	.2988E-15
-.1	.8328E-03	.8334E-02	.8328E-03	.1000E-01	.2026E-15	.2090E-15
.0	.8329E-03	.8334E-02	.8329E-03	.1000E-01	.1766E-15	.1846E-15
.1	.8328E-03	.8334E-02	.8328E-03	.1000E-01	.1319E-15	.1383E-15
.2	.8326E-03	.8335E-02	.8326E-03	.1000E-01	.2288E-15	.2281E-15
.3	.8323E-03	.8335E-02	.8323E-03	.1000E-01	.4405E-15	.4172E-15
.4	.8319E-03	.8336E-02	.8319E-03	.1000E-01	.8094E-15	.7174E-15
.5	.8312E-03	.8338E-02	.8312E-03	.1000E-01	.1608E-14	.1311E-14
.6	.8304E-03	.8339E-02	.8304E-03	.1000E-01	.3523E-14	.2610E-14
.7	.8293E-03	.8342E-02	.8293E-03	.1000E-01	.8555E-14	.5753E-14
.8	.8280E-03	.8344E-02	.8280E-03	.1000E-01	.2230E-13	.1345E-13
.9	.8265E-03	.8347E-02	.8265E-03	.1000E-01	.6440E-13	.3503E-13
1.0	.8246E-03	.8351E-02	.8246E-03	.1000E-01	.2094E-12	.1039E-12
1.1	.8222E-03	.8356E-02	.8222E-03	.1000E-01	.7802E-12	.3571E-12
1.2	.8191E-03	.8362E-02	.8191E-03	.1000E-01	.3431E-11	.1466E-11
1.3	.8147E-03	.8371E-02	.8147E-03	.1000E-01	.1860E-10	.7485E-11
1.4	.8079E-03	.8385E-02	.8079E-03	.1000E-01	.1326E-09	.5047E-10
1.5	.7969E-03	.8407E-02	.7969E-03	.1000E-01	.1375E-08	.4946E-09
1.6	.7765E-03	.8448E-02	.7765E-03	.1000E-01	.2478E-07	.8311E-08
1.7	.7321E-03	.8538E-02	.7321E-03	.1000E-01	.1102E-05	.3305E-06

Table for optimal β's, their row-sum and the square of the norm of local truncation error functionals in $H^2(C_r)$-space for Cowell's usual 3-point method and the corresponding β-optimal method, interpolatory for exp(±1.6x) at the nodal points with r=2.01, a=-1.8, b=1.8, n=36, h=.1; $\alpha_0=-1$, $\alpha_1=2$, $\alpha_3=-1$; $\beta_0=.083333$, $\beta_1=.833333$, $\beta_2=.083333$.

Table - 7b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.257124E-04
2	2	.610703E-04	2	.236998E-04
3	3	.430195E-03	2	.668193E-04
4	2	.133292E-03	2	.263115E-04
5	2	.348263E-03	2	.241046E-04
6	3	.127772E-03	2	.307981E-04
7	2	.313175E-04	2	.751404E-05
8	2	.133523E-03	2	.145138E-04
9	2	.735570E-04	2	.795490E-05
10	1	.170782E-02	1	.386341E-03
11	1	.738872E-03	1	.511681E-03
12	1	.718937E-03	1	.507192E-03
13	2	.298705E-05	2	.105352E-05
14	2	.167071E-05	2	.459325E-06
15	2	.392662E-05	2	.154223E-05
16	2	.236517E-05	2	.756348E-06
17	1	.257920E-07	1	.708103E-08
18	1	.151826E-06	1	.167395E-07
19	3	.509406E-03	2	.106010E-03
20	3	.464907E-03	2	.961642E-04
21	2	.304135E-03	2	.232490E-04
22	2	.208304E-03	2	.149971E-04
23	2	.300455E-03	2	.438887E-04
24	2	.287372E-04	2	.613905E-05

Table for number of iterations for convergence of the solution and the average discretisation error using Cowell's 3-points usual and the corresponding β-optimal method in $H^2(C_r)$ space, interpolatory for functions exp(±1.6x), for 24 BVP-s.

The results of Table 7c are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1 for IVP's with equations 1-9 and 19-24, and with r=2.7, a=-1.4, b=1.4, n=28, h=.1 for IVP's with equations 10-18. Table 7c reveals that as compared to usual method β-optimal method interpolatory for linearly independent functions exp (±1.6x) for IVP is one decimal place better on equations 1,2,4-13 16-24; and just better on equations 3,14 and 15.

Table - 7c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.172832E-02
2	4	.250457E-02	3	.676315E-03
3	8	.760039E-01	5	.120006E-01
4	5	.132805E-01	4	.116489E-02
5	4	.716823E-02	3	.301960E-03
6	5	.356402E-02	4	.915038E-03
7	4	.354625E-03	3	.925088E-04
8	4	.211573E-02	3	.278186E-03
9	3	.604542E-03	3	.806865E-04
10	4	.119641E-01	4	.725326E-02
11	4	.130464E+00	4	.269349E-01
12	4	.129361E+00	4	.262629E-01
13	2	.128426E-05	2	.720024E-06
14	2	.831124E-06	2	.469907E-06
15	2	.193794E-05	2	.104693E-05
16	2	.130401E-05	2	.683572E-06
17	1	.456442E-08	1	.891521E-09
18	1	.343343E-07	1	.242165E-08
19	11	.103867E+00	6	.180424E-01
20	4	.188589E-02	3	.436142E-03
21	4	.112364E-02	3	.117028E-03
22	5	.115497E-01	4	.108422E-02
23	4	.610397E-02	3	.631845E-03
24	3	.542588E-04	2	.955502E-05

Table for number of iterations for convergence of the solution and the average discretisation error for using Cowell's usual method with function evaluation at three points and the corresponding β-optimal method in $H^2(C_r)$-space, interpolatory for linearly independent functions exp(±1.6x) applied on 24 IVP-s.

In Figures to follow, we are using the following notations.

Beta-Optimal(1) : β-optimal method

Beta-Optimal(2) : β-optimal method with restriction

Beta-Optimal(3) : β-optimal method interpolatory for polynomials of degree 3.

Beta-Optimal(4) : β-optimal method interpolatory for exp(±1.6x).

All the above beta-optimal methods are corresponding to Cowell's usual method with function evaluation at three points.

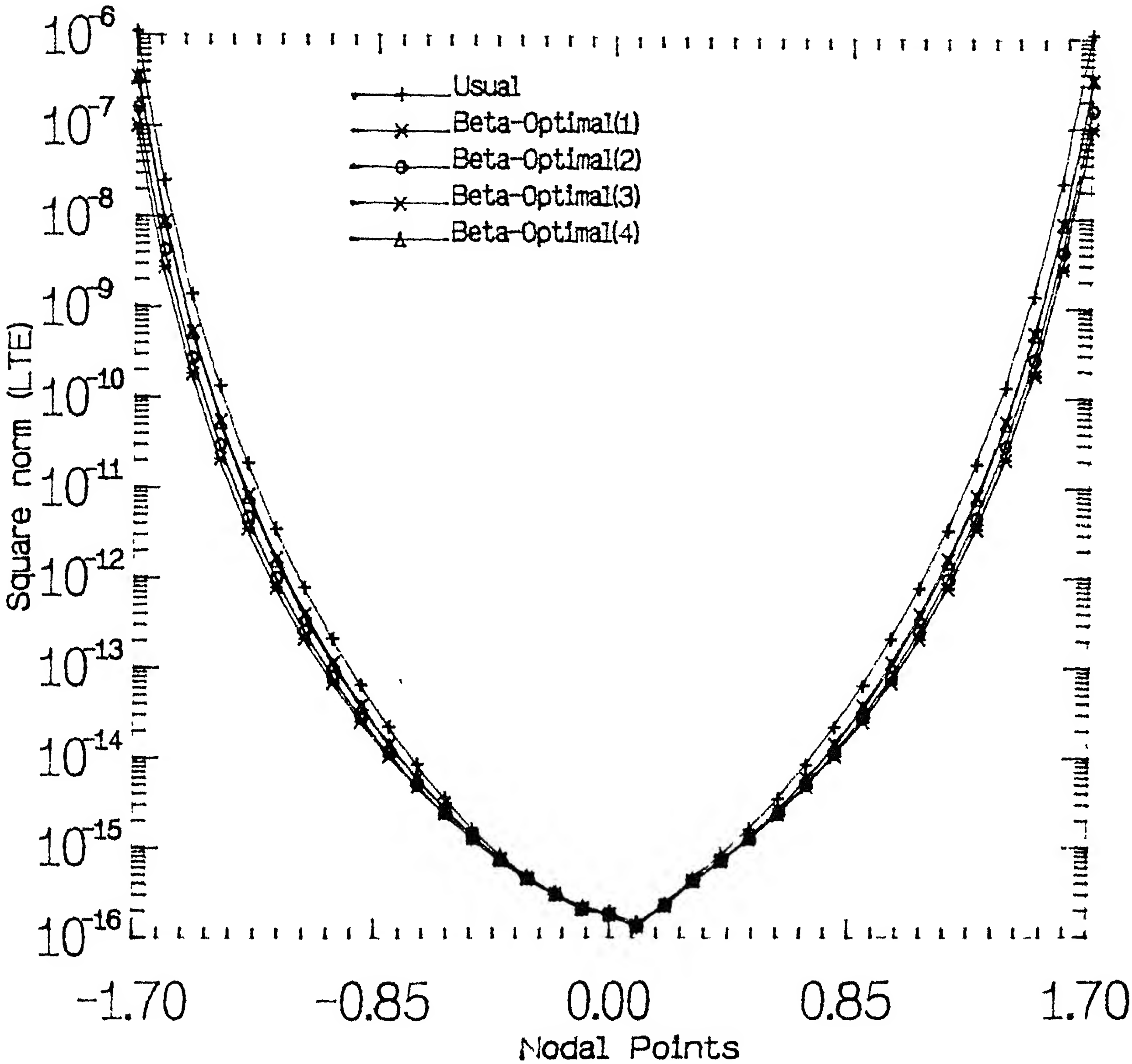
Beta-Optimal(3) : β-optimal method interpolatory for polynomials of degree 3.

Beta-Optimal(4) : β-optimal method interpolatory for exp(±1.6x).

All the above beta-optimal methods are corresponding to Cowell's usual method with function evaluation at three points.

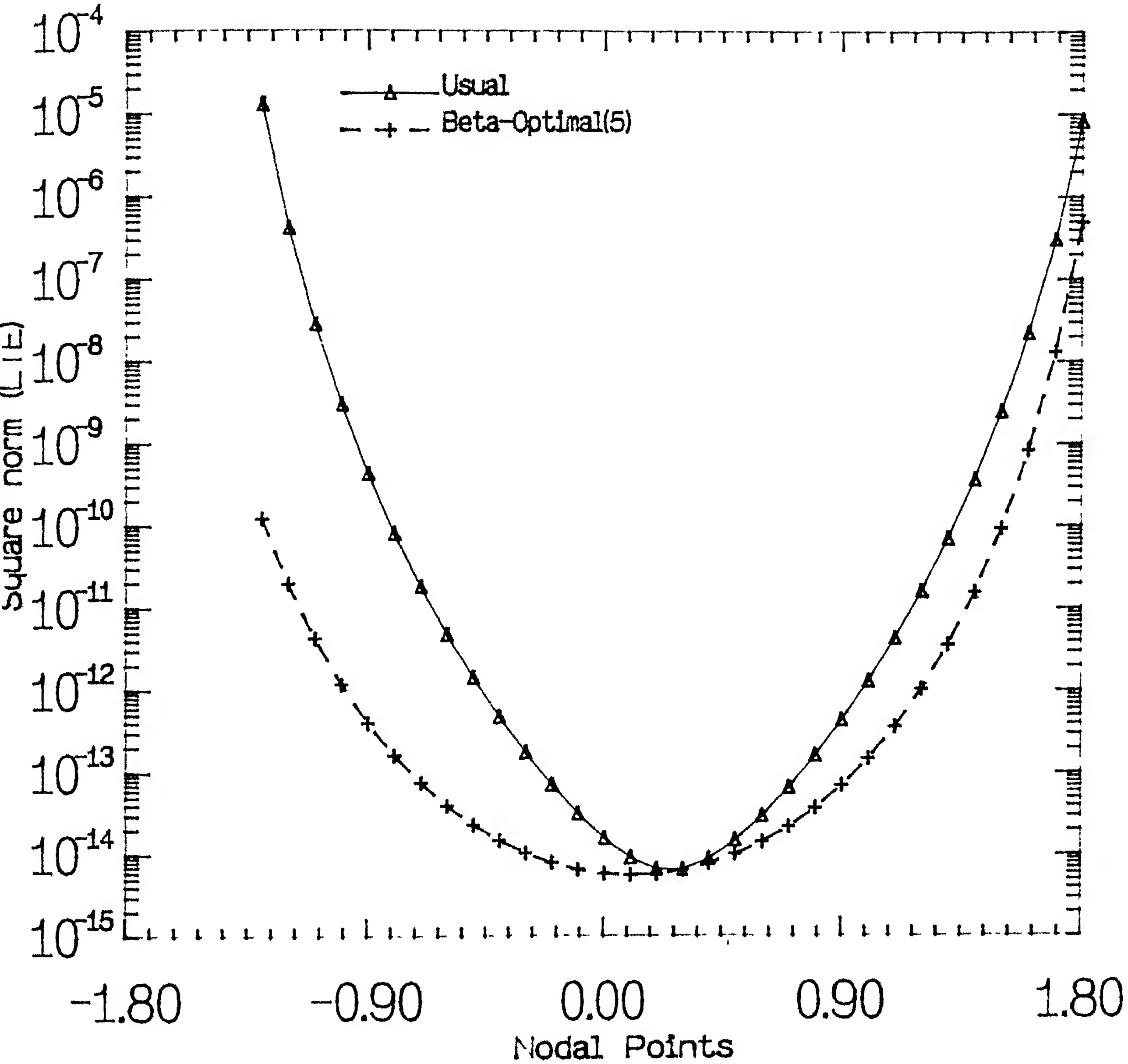
Beta-Optimal(5) : β-optimal method corresponding to Stormer's usual method with function evaluation at five points.

The following graphs are drawn according to the corresponding tabular results given earlier. Figure 1 is drawn from the tabular results given in Tables 2a, 5a, 6a and 7a. Figure 2 is drawn from the tabular results given in Table 3a. Figure 3 is drawn from the tabular results given in Table 4a. Figure 1 shows that the β-optimal method is giving more optimized results than other optimal methods. From figure 3, we conclude that α-optimal method is not giving so promising results, and even though the numerical calculations are done in double precision, near the origin, the square norm of local truncation errors being of the order of 10^{-16} or 10^{-17}, these results are not very reliable.



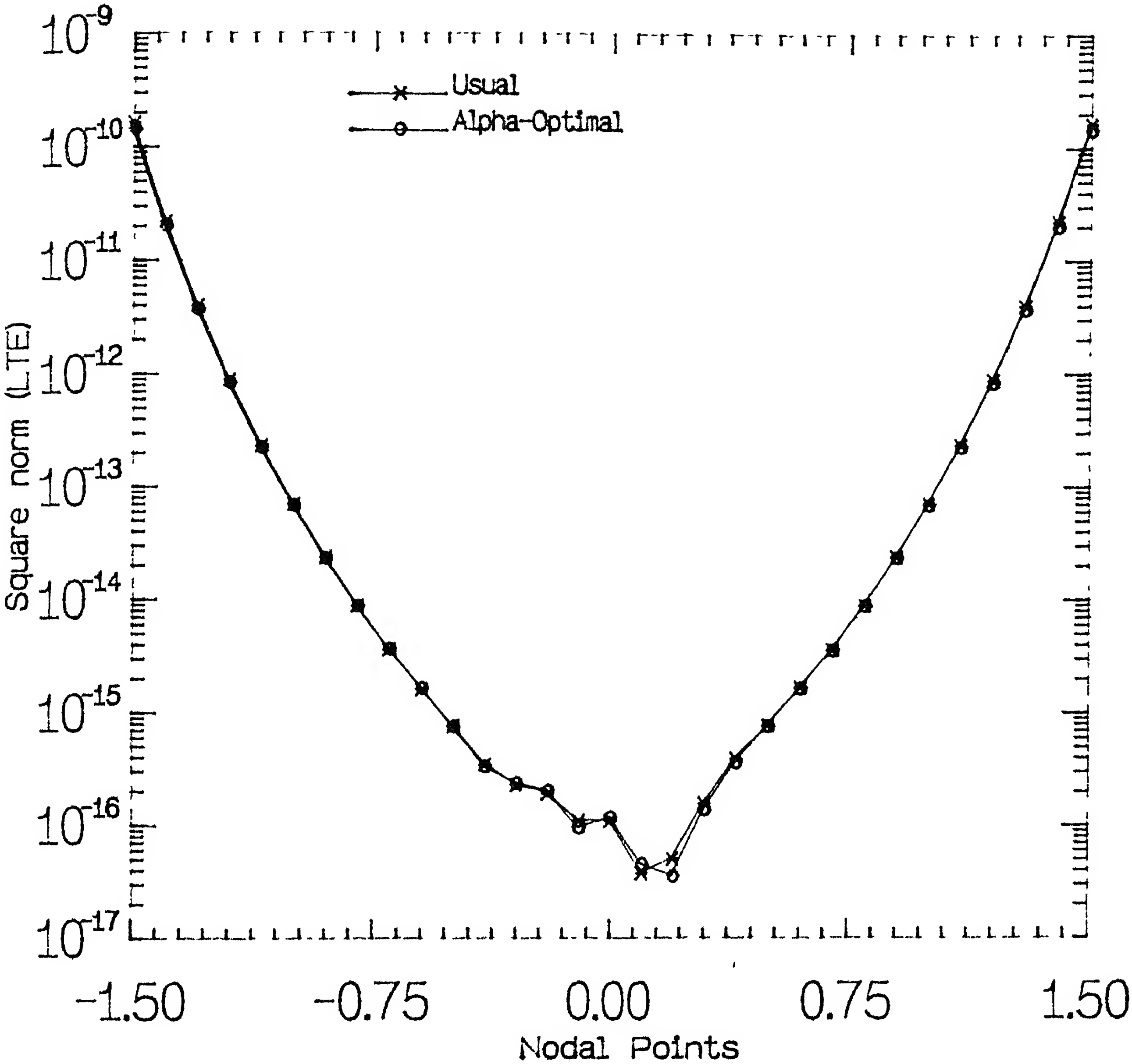
Square of norm of local truncation error in $H^2(C_r)$-space

FIG. 1



Square of norm of local truncation error in $H^2(C_r)$-space

FIG. 2



Square of norm of local truncation error in $H^2(C_\gamma)$-space

FIG. 3

4.6 Behavior of the Coefficients As $r \to \infty$

From Tables we observe that the coefficients of β-optimal multistep methods, β-optimal multistep methods interpolatory for polynomials of certain degree or interpolatory for linearly independent arbitrary functions are approximately the same as the corresponding coefficients of the usual method at the points under consideration in a neighborhood of the center of the circle C_r, which in other words are the points that are well inside the domain of the space. Such a kind of property of the coefficients has been discussed in [16], [82], [113], [154] and [158]. For the space $H^2(C_r)$, the behavior of the coefficients in the quadrature formulae as $r \to \infty$ is studied by Barnhill [16], Kaul [113] and Finmay and Price Jr. [82] and a similar study for the optimal multistep methods for first order differential equations is done by Brij Bhusan [27]. Here we obtain the corresponding results for the optimal multistep methods in $H^2(C_r)$ space for the second order differential equations.

Theorem 11: Let

(18) $$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j^F f_{n+k-j} = 0$$

be a multistep method interpolatory for functions $\left\{\phi_{\delta_{t0}}, \ldots, \phi_k\right\}$ and let the matrix $[\phi_i''(x_{n+k-j})]_{i,j=\delta_{t0}(1)k}$ be nonsingular. Let

(19) $$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,r}^F f_{n+k-j} = 0$$

be an optimal multistep formula in $H^2(C_r)$ space, interpolatory for

functions $\left\{\phi_{\delta_{t0}},\ldots,\phi_{p-1+\delta_{t0}}\right\}$, $0 \le p \le k+\delta_{t1} = k+1-\delta_{t0}$, ($p = 0$ implies non-interpolatory case for these functions). If the local truncation error functional $\hat{T}^F_{nr}$ for (19) satisfies

$$\text{(20)} \qquad \lim_{r\to\infty} \hat{T}^F_{nr}(\phi_j) = 0, \qquad j = p+\delta_{t0}(1)k,$$

then

$$\text{(21)} \qquad \lim_{r\to\infty} \hat{\beta}^F_{j,r} = \beta^F_j, \qquad j = \delta_{t0}(1)k.$$

<u>Proof:</u> For the errors for the functions $\phi_{\delta_{t0}},\phi_{\delta_{t0+1}},\ldots,\phi_k$ in (18) and (19) we get

$$\text{(22)} \qquad \sum_{j=0}^{k} \alpha_j \phi_i(x_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \beta^F_j \phi''_i(x_{n+k-j}) = 0, \qquad i = \delta_{t0}(1)k,$$

and

$$\text{(23)} \qquad \sum_{j=0}^{k} \alpha_j \phi_i(x_{n+k-j}) - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} \phi''_i(x_{n+k-j}) = \hat{T}^F_{nr}(\phi_i), \; i= \delta_{t0}(1)k.$$

Subtracting (23) from (22), we get

$$- h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} \phi''_i(x_{n+k-j}) + h^2 \sum_{j=\delta_{t0}}^{k} \beta^F_j \phi''_i(x_{n+k-j}) = \hat{T}^F_{nr}(\phi_i), \; i = \delta_{t0}(1)k.$$

In matrix notation, we have

$$\text{(24)} \qquad h^2 G\hat{B}^F_r - h^2 GB^F + \hat{T}^F_{nr} = 0,$$

where

$$G = [\phi''_i(x_{n+k-j})]_{i,j=\delta_{t0}(1)k},$$

$$\hat{B}^F_r = \left[\hat{\beta}^F_{\delta_{t0},r},\hat{\beta}^F_{\delta_{t0}+1,r},\ldots,\hat{\beta}^F_{k,r}\right]^T,$$

$$B^F = \left[\beta^F_{\delta_{t0}},\beta^F_{\delta_{t0}+1},\ldots,\beta^F_k\right]^T,$$

and $$\hat{T}^F_{nr} = \left[\hat{T}^F_{nr}(\phi_{\delta_{t0}}),\hat{T}^F_{nr}(\phi_{\delta_{t0}+1}),\ldots,\hat{T}^F_{nr}(\phi_k)\right]^T.$$

Since the optimal method (19) is interpolatory for $\phi_{\delta_{t0}},\ldots,\phi_{p-1+\delta_{t0}}$

$$\hat{T}^F_{nr}(\phi_{\delta_{t0}}) = \ldots\ldots = \hat{T}^F_{nr}(\phi_{p+\delta_{t0}-1}) = 0$$

by (20), $\lim_{r\to\infty} \hat{T}^F_{nr} = 0$. Since G is nonsingular, we get from (24)

$$\lim_{r\to\infty} \hat{B}^F_r = \lim_{r\to\infty} B^F$$

or, $$\lim_{r\to\infty} \hat{\beta}^F_{j,r} = \beta^F_j, \quad j = \delta_{t0}(1)k.$$ Hence the proof.

<u>Theorem 12</u>: Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k}\alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Then, the $H^2(C_r)$-coefficients $\hat{\beta}_{j,r}$ of an optimal multistep method

$$\sum_{j=0}^{k}\alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} f_{n+k-j} = 0, \tag{25}$$

approach the coefficients β_j of the usual multistep method

$$\sum_{j=0}^{k}\alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0 \tag{26}$$

of maximal polynomial precision.

<u>Proof:</u> Since the usual method (26) is interpolatory for polynomials of maximal degree and it is assumed that α_j's are known constants with $\sum_{j=0}^{k}\alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$, the coefficients β_j's of the usual method (26) can uniquely be determined by using that it is interpolatory for polynomials $x^2, x^3, \ldots, x^{k+\delta_{t1}+1}$. In view of Theorem 1, we need to prove that the local truncation error functional $\hat{T}_{nr}$ for the optimal method (25) satisfies

$$\lim_{r\to\infty} \hat{T}_{nr}\,(x^i) = 0, \qquad 0 \le i \le k+\delta_{t1}+1$$

If T_n is the local truncation error functional for the usual method then in the space of optimization, e.g. in $H^2(C_r)$ space we have

$$\|\hat{T}_{nr}\| \le \|T_n\|.$$

Since $\{\psi_k\}_{k=0}^{\infty}$ is a complete orthonormal sequence in $H^2(C_r)$ space, where $\psi_k(z) = \dfrac{z^k}{\sqrt{2\pi r}\, r^k}$, $k \ge 0$; and $T_n(x^j) = 0$, $0 \le j \le k+\delta_{t1}+1$,

$$\sum_{i=0}^{\infty} |\hat{T}_{nr}(\psi_i)|^2 \le \sum_{j=0}^{\infty} |T_n(\psi_j)|^2 = \sum_{j=k+\delta_{t1}+2}^{\infty} \frac{1}{2\pi}\, r^{-(2j+1)}\, |T_n(x^j)|^2$$

or, $$\sum_{i=0}^{\infty} \frac{1}{2\pi}\, r^{-(2i+1)}\, |\hat{T}_{nr}(x^i)|^2 \le \sum_{j=k+\delta_{t1}+2}^{\infty} \frac{1}{2\pi}\, r^{-(2j+1)}\, |T_n(x^j)|^2$$

Thus for each fixed i, $0 \le i \le k+\delta_{t1}+1$,

$$|\hat{T}_{nr}(x^i)|^2 \le \sum_{j=k+\delta_{t1}+2}^{\infty} r^{-2(j-i)}\, |T_n(x^j)|^2.$$

The expression on the right hand side approaches zero as $r \to \infty$.

So, $$\lim_{r\to\infty} \hat{T}_{nr}\,(x^i) = 0, \qquad 0 \le i \le k+\delta_{t1}+1.$$

Hence the result.

<u>Theorem 13:</u> Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k} \alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Then the $H^2(C_r)$-coefficients $\hat{\beta}^{P}_{j,r}$ of the optimal multistep method

$$(27) \qquad \sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^{P}_{j,r}\, f_{n+k-j} = 0,$$

interpolatory for polynomials of degree $p \le k+\delta_{t1}+1$, approach as $r \to \infty$, the coefficients β_j of the corresponding multistep method of highest degree polynomial precision

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0.$$

<u>Proof:</u> Since $\sum_{j=0}^{k} \alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$, the method (27) is interpolatory for constants and x. As it is interpolatory for polynomials of degree p, the local truncation error functional $\hat{T}^P_{nr}$ of (27) satisfies

$$\hat{T}^P_{nr}(x^i) = 0, \quad 0 \le i \le p.$$

In view of Theorem 11, it is sufficient to prove that

$$\lim_{r\to\infty} \hat{T}^P_{nr}(x^i) = 0, \quad p+1 \le i \le k+\delta_{t1}+1.$$

If T_n denotes the local truncation error functional of the usual method, then in the space of optimization viz. in $H^2(C_r)$-space

$$\|\hat{T}^P_{nr}\| \le \|T_n\|.$$

As given in Theorem 12,

$$\sum_{i=0}^{\infty} |\hat{T}^P_{nr}(\psi_i)|^2 \le \sum_{j=0}^{\infty} |T_n(\psi_j)|^2 = \sum_{j=k+\delta_{t1}+2}^{\infty} \frac{1}{2\pi} r^{-(2j+1)} |T_n(x^j)|^2.$$

Since $\hat{T}^P_{nr}(x^i) = 0$, for $0 \le i \le p$, for $i \ge p+1$, we get

$$|\hat{T}^P_{nr}(x^i)|^2 \le \sum_{j=k+\delta_{t1}+2}^{\infty} r^{-2(j-i)} |T_n(x^j)|^2.$$

The expression on the right approaches zero as $r\to\infty$, for $i \le k+\delta_{t1}+1$. Hence

$$\lim_{r \to \infty} \hat{T}_{nr}(x^l) = 0, \qquad p+1 \le l \le k+\delta_{t1}+1$$

Hence the result.

<u>Theorem 14</u>: Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k} \alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Let the $(k+\delta_{t1})x(k+\delta_{t1})$ matrix M be nonsingular, where

$$M = \begin{bmatrix} \phi_1''(x_{n+k-1+\delta_{t1}}) \cdots\cdots\cdots\cdots \phi_1''(x_n) \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ \phi_p''(x_{n+k-1+\delta_{t1}}) \cdots\cdots\cdots\cdots \phi_p''(x_n) \\ 1 \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots 1 \\ x_{n+k-1+\delta_{t1}} \cdots\cdots\cdots\cdots\cdots\cdots x_n \\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots \\ x_{n+k-1+\delta_{t1}}^{k-p-\delta_{t0}} \cdots\cdots\cdots\cdots x_n^{k-p-\delta_{t0}} \end{bmatrix}.$$

Then the coefficients $\hat{\beta}^F_{k-j,r}$'s in $H^2(C_r)$ space of the optimal multistep method

$$\text{(28)} \qquad \sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} f_{n+k-j} = 0,$$

interpolatory for functions $\{\phi_1, \phi_2, \ldots, \phi_p\}$, $p \le k+\delta_{t1}$ approach the coefficients β^F_j 's of the unique multistep method

$$\text{(29)} \qquad \sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta^F_j f_{n+k-j} = 0,$$

which is interpolatory for functions

$$\{\phi_1, \phi_2, \ldots, \phi_p, x^2, x^3, \ldots, x^{k+\delta_{t1}+1-p}\}.$$

<u>Proof:</u> As the matrix M is non-singular, for given α_j's, β^F_j 's of the method (29) can be determined uniquely. Since both the methods

are interpolatory for functions $\{\phi_1,\phi_2,\ldots,\phi_p\}$, by Theorem 11, it is sufficient to prove that the local truncation error functional $\hat{T}^F_{nr}$ of (28) satisfies

$$\lim_{r\to\infty} \hat{T}^F_{nr}\,(x^i) = 0, \qquad 2 \le i \le k+\delta_{t1}+1-p.$$

Since $\sum_{j=0}^{k}\alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$, the usual method (29) is exact for constants and x. Also it is exact for x^2, $x^3,\ldots,x^{k+\delta_{t1}+1-p}$. If T^F_n is the local truncation error functional of the usual method (29), then $T^F_n(x^i) = 0$, for $0 \le i \le k+\delta_{t1}+1-p$. As in Theorem 12,

$$\sum_{i=0}^{\infty} |\hat{T}^F_{nr}(\psi_i)|^2 \le \sum_{j=0}^{\infty} |T^F_n(\psi_j)|^2 = \sum_{j=k+\delta_{t1}+2-p}^{\infty} \frac{1}{2\pi}\, r^{-(2j+1)}\, |T^F_n(x^j)|^2$$

or, $$\sum_{i=0}^{\infty} \frac{1}{2\pi}\, r^{-(2i+1)}\, |\hat{T}^F_{nr}(x^i)|^2 \le \sum_{j=k+\delta_{t1}+2-p}^{\infty} \frac{1}{2\pi}\, r^{-(2j+1)}\, |T^F_n(x^j)|^2.$$

Thus for each fixed i, $i \ge 0$

$$|\hat{T}_{nr}(x^i)|^2 \le \sum_{j=k+\delta_{t1}+2-p}^{\infty} r^{-2(j-i)}\, |T_n(x^j)|^2.$$

For $2 \le i \le k+\delta_{t1}+1-p$, the expression on the right hand side approaches zero as $r \to \infty$. Hence

$$\lim_{r\to\infty} \hat{T}^F_{nr}(x^i) = 0, \quad 2 \le i \le k+\delta_{t1}+1-p.$$

Hence the result.

4.7 An Asymptotic Estimate of Local Truncation Error

In this section, we shall give asymptotic estimate of the optimal β-coefficients and the local truncation error functionals

in $H^2(C_r)$ space, for both the usual and the β-optimal methods and compare them in some simple cases. First, we shall consider Stormer's method with function evaluation at one point. Next, we shall consider Cowell's method with function evaluation at three points as the usual method. For solving numerically a differential equation, with some initial or boundary conditions, of the form

$$\text{(I)} \qquad y'' = f(x,y),$$

Stormer's usual method with function evaluation at one point is

$$\text{(30)} \qquad \sum_{i=0}^{2} \alpha_i y_{n-1+i} + h^2 f_n = 0,$$

where $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; the corresponding β-optimal method is

$$\text{(31)} \qquad \sum_{i=0}^{2} \alpha_i y_{n-1+i} + h^2 \hat{\beta}_{1,n} f_n = 0.$$

The normal equation for obtaining $\hat{\beta}_{1,n}$ is given by

$$\sum_{j=0}^{2} \alpha_j D2(x_{n-1+j}, \bar{x}_n) + h^2 \hat{\beta}_{1,n} D2''(x_n, \bar{x}_n) = 0,$$

so that
$$\hat{\beta}_{1,n} = -\frac{1}{h^2} \frac{\sum_{j=0}^{2} \alpha_j D2(x_{n-1+j}, \bar{x}_n)}{D2''(x_n, \bar{x}_n)}.$$

Using the definitions of $D2(x_{n-1+j}, \bar{x}_n)$ and $D2''(x_n, \bar{x}_n)$ from (5) and (6), as in the Case 1 of Lemma 5 of Chapter 3,

$$\text{(32)} \qquad \hat{\beta}_{1,n} = C \left[\frac{(x-h)^2 (r^2 - x^2)^3}{(r^2 - x^2 + xh)^3} + \frac{(x+h)^2 (r^2 - x^2)^3}{(r^2 - x^2 - xh)^3} - 2x^2 \right]$$

with $x_n = x$, and $C = \dfrac{(r^2 - x^2)^2}{2h^2(r^4 + 4r^2x^2 + x^4)}$. Hence

$$\hat{\beta}_{1,n} = C\left[(x-h)^2 \left\{ 1 + \frac{hx}{r^2 - x^2} \right\}^{-3} + (x+h)^2 \left\{ 1 - \frac{hx}{r^2 - x^2} \right\}^{-3} - 2x^2 \right]$$

$$= 2h^2\ C\ \left[1+\frac{6x^2}{r^2-x^2}+\frac{6x^2(x^2+h^2)}{(r^2-x^2)^2}+\frac{20h^2x^4}{(r^2-x^2)^3}+\frac{15h^2x^4(x^2+h^2)}{(r^2-x^2)^4}\right.$$

$$\left.+\frac{42h^4x^6}{(r^2-x^2)^5}+\cdots\cdots\cdots\cdots\right].$$

It follows that

$$(33)\quad \hat{\beta}_{1,n} = 1 + \frac{(r^2-x^2)^2}{(r^4+4r^2x^2+x^4)}\left\{\frac{6x^2h^2}{(r^2-x^2)^2}+\frac{20x^4h^2}{(r^2-x^2)^3}+\frac{15x^6h^2}{(r^2-x^2)^4}\right.$$

$$+\frac{15x^4h^4}{(r^2-x^2)^4}+\frac{42x^6h^4}{(r^2-x^2)^5}+\frac{28x^8h^4}{(r^2-x^2)^6}+\frac{28x^6h^6}{(r^2-x^2)^6}+\frac{72x^8h^6}{(r^2-x^2)^7}+\frac{45x^{10}h^6}{(r^2-x^2)^8}+$$

$$\left.\frac{45x^8h^8}{(r^2-x^2)^8}+\frac{110x^{10}h^8}{(r^2-x^2)^9}+\frac{66x^{12}h^8}{(r^2-x^2)^{10}}+\cdots\cdots\right\}.$$

We see that $\hat{\beta}_{1n}-1$ is precisely of order h^2 at a fixed $x \neq 0$; at $x = 0$, $\hat{\beta}_{1n} = 1$, and if $x = O(h)$, then $\hat{\beta}_{1n} - 1 = O(h^4)$. Square norm of local truncation error functional for optimal method (31), is given by

$$\|\hat{T}_n\|^2 = \sum_{i=0}^{2}\bar{\alpha}_i\left(\sum_{j=0}^{2}\alpha_j K(x_{n-1+j},\bar{x}_{n-1+i}) + h^2\hat{\beta}_{1,n}\overline{D2(x_{n-1+i},\bar{x}_n)}\right).$$

As α_i's and the nodal points are real, putting $x_n = x$, and using values of $K(x_{n-1+j},\bar{x}_{n-1+i})$, $D2(x_{n-1+i},\bar{x}_n)$ from (4) and (5), we get

$$\|\hat{T}_n\|^2 = \sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\alpha_j\frac{r}{2\pi(r^2-x_{n-1+j}x_{n-1+i})} + h^2\hat{\beta}_{1,n}\sum_{i=0}^{2}\alpha_i\frac{rx_{n-1+i}^2}{\pi(r^2-x_{n-1+i}x_n)^3}.$$

Writing $x_n = x$, and substituting the values of α_j's, we get

$$(34)\quad \|\hat{T}_n\|^2 = \frac{r}{\pi}\sum_{i=0}^{2}\alpha_i\left[\frac{-1}{2(r^2-(x-h)(x-(1-i)h))}+\frac{2}{2(r^2-x(x-(1-i)h))}\right.$$

$$\left.+\frac{-1}{2(r^2-(x+h)(x-(1-i)h))}\right]+\frac{r}{\pi}h^2\hat{\beta}_{1,n}\sum_{i=0}^{2}\alpha_i\frac{(x-(1-i)h)^2}{(r^2-x(x-(1-i)h))^3}.$$

Square norm of local truncation error functional for usual method

(30), is given by

$$\|T_n\|^2 = \sum_{i=0}^{2}\bar{\alpha}_i\left(\sum_{j=0}^{2}\alpha_j K(x_{n-1+j},\bar{x}_{n-1+i}) + h^2\overline{D2(x_{n-1+i},\bar{x}_n)}\right)$$

$$+ h^2\left(\sum_{j=0}^{2}\alpha_j D2(x_{n-1+j},\bar{x}_n) + h^2 D2''(x_n,\bar{x}_n)\right).$$

Putting $x_n = x$ and using values of $K(x_{n-1+j},\bar{x}_{n-1+i})$, $D2(x_{n-1+i},\bar{x}_n)$ from (4) and (5), we get

$$(35) \qquad \|T_n\|^2 = \sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\alpha_j\frac{r}{2\pi[r^2-\{x-(1-j)h\}\{x-(1-i)h\}]}$$

$$+h^2\sum_{i=0}^{2}\alpha_i\frac{r\{x-(1-i)h\}^2}{\pi[r^2-\{x-(1-i)h\}x]^3}+h^2\sum_{j=0}^{2}\alpha_j\frac{r\{x-(1-j)h\}^2}{\pi[r^2-\{x-(1-j)h\}x]^3}$$

$$+ h^4\frac{2r}{\pi(r^2-x^2)^5}[r^2(r^2+4x^2)+x^4].$$

(i) <u>At $x = 0$</u>:

From (32), $\left.\hat{\beta}_{1,n}\right|_{x=0} = \frac{1}{2h^2}\frac{2h^2}{r^6}\frac{r^{10}}{r^4} = 1.$ From (34) and (35),

$$\left.\|\hat{T}_n\|^2\right|_{x=0} = \frac{r}{\pi}\sum_{i=0}^{2}\alpha_i\left\{\left(\frac{-1}{2(r^2-h^2(1-i))}+\frac{2}{2r^2}+\frac{-1}{2(r^2+h^2(1-i))}\right)+\frac{h^4}{r^6}(1-i)^2\right\},$$

and

$$\left.\|T_n\|^2\right|_{x=0} = \frac{r}{\pi}\sum_{i=0}^{2}\alpha_i\left\{\left(\frac{-1}{2(r^2-h^2(1-i))}+\frac{2}{2r^2}+\frac{-1}{2(r^2+h^2(1-i))}\right)+\frac{h^4}{r^6}(1-i)^2\right\}$$

$$+\frac{r}{\pi}\frac{h^4}{r^6}\sum_{j=0}^{2}\alpha_i(1-j)^2 + \frac{r}{\pi}\frac{2h^4}{r^6}$$

$$= \left.\|\hat{T}_n\|^2\right|_{x=0} - \frac{r}{\pi}\frac{2h^4}{r^6} + \frac{r}{\pi}\frac{2h^4}{r^6}.$$

Hence, $\left.\|T_n\|^2\right|_{x=0} = \left.\|\hat{T}_n\|^2\right|_{x=0}$, which is otherwise also clear as $\hat{\beta}_{1n}=1$.

(ii) <u>At x = h:</u>

From (32), we get

$$\hat{\beta}_{1,n}\Big|_{x=h} = \frac{(r^2 - h^2)^2 . (r^6 - 6r^2h^4 + 6h^6)}{(r^2 - 2h^2)^3 . (r^4 + 4r^2h^2 + h^4)}. \tag{36}$$

From (34),

$$\|\hat{T}_n\|^2\Big|_{x=h} = \frac{r}{\pi} \sum_{i=0}^{2} \alpha_i \left[\left\{-\frac{1}{2r^2} + \frac{1}{(r^2-ih^2)} - \frac{1}{2(r^2-2ih^2)}\right\} + \hat{\beta}_{1,n}\frac{i^2h^4}{(r^2-ih^2)^3}\right]$$

$$= \frac{r}{\pi} (A + B), \text{ say.}$$

Let

$$A_1 = \sum_{i=0}^{2} \alpha_i \left(-\frac{1}{2r^2}\right) = 0,$$

$$A_2 = \sum_{i=0}^{2} \alpha_i \frac{1}{(r^2-ih^2)} = -\frac{1}{r^2} + \frac{2}{(r^2-h^2)} - \frac{1}{(r^2-2h^2)},$$

and $$A_3 = \sum_{i=0}^{2} \alpha_i \frac{-1}{2(r^2-2ih^2)} = \frac{1}{2r^2} - \frac{1}{(r^2-2h^2)} + \frac{1}{2(r^2-4h^2)}.$$

Then $$A = A_1 + A_2 + A_3 = \frac{2}{(r^2-h^2)} - \frac{2}{(r^2-2h^2)} + \frac{1}{2(r^2-4h^2)} - \frac{1}{2r^2}$$

$$= \frac{2}{r^2}\left(1 - \frac{h^2}{r^2}\right)^{-1} - \frac{2}{r^2}\left(1 - \frac{2h^2}{r^2}\right)^{-1} + \frac{1}{2r^2}\left(1 - \frac{4h^2}{r^2}\right)^{-1} - \frac{1}{2r^2}.$$

So,

$$A = \frac{2}{r^2}\left(\frac{h^4}{r^4}+\frac{h^6}{r^6}+\frac{h^8}{r^8}+\frac{h^{10}}{r^{10}}+\frac{h^{12}}{r^{12}}+\ldots\right) - \frac{2}{r^2}\left(8\frac{h^6}{r^6}+16\frac{h^8}{r^8}+32\frac{h^{10}}{r^{10}}+64\frac{h^{12}}{r^{12}}+\ldots\right) \tag{37}$$

$$+ \frac{1}{2r^2}\left(64\frac{h^6}{r^6}+256\frac{h^8}{r^8}+1024\frac{h^{10}}{r^{10}}+4096\frac{h^{12}}{r^{12}}+\ldots\right).$$

$$B = h^4\hat{\beta}_{1,n} \sum_{i=0}^{2} \alpha_i \frac{i^2}{(r^2-ih^2)^3} = h^4\hat{\beta}_{1,n}\left(\frac{2}{(r^2-h^2)^3} - \frac{4}{(r^2-2h^2)^3}\right)$$

$$= 2h^4 \frac{(r^2 - h^2)^2.(r^6 - 6r^2h^4 + 6h^6)}{(r^2 - 2h^2)^3.(r^4 + 4r^2h^2 + h^4)} \left(\frac{-r^6 + 6r^2h^4 - 6h^6}{(r^2-h^2)^3(r^2-2h^2)^3}\right)$$

$$= -2h^4 (r^6-6r^2h^4+6h^6)^2 \frac{1}{r^{12}}\left(1-\frac{2h^2}{r^2}\right)^{-6}\frac{1}{r^4}\left[1+\frac{h^2}{r^2}\left(4+\frac{h^2}{r^2}\right)\right]^{-1}\frac{1}{r^2}\left[1-\frac{h^2}{r^2}\right]^{-1}$$

$$= -\frac{2}{r^2}\frac{h^4}{r^4}\left(1-\frac{6h^4}{r^4}+\frac{6h^6}{r^6}\right)^2\left[1-\frac{h^2}{r^2}\right]^{-1}\left(1-\frac{2h^2}{r^2}\right)^{-6}\left[1+\frac{h^2}{r^2}\left(4+\frac{h^2}{r^2}\right)\right]^{-1}$$

$$= -\frac{2}{r^2}\frac{h^4}{r^4}\left(1-12\frac{h^4}{r^4}+12\frac{h^6}{r^6}+36\frac{h^8}{r^8}+\dots\right).\left(1+\frac{h^2}{r^2}+\frac{h^4}{r^4}+\frac{h^6}{r^6}+\frac{h^8}{r^8}+\dots\right).$$

$$\left(1+12\frac{h^2}{r^2}+84\frac{h^4}{r^4}+448\frac{h^6}{r^6}+2016\frac{h^8}{r^8}+..\right).\left(1-4\frac{h^2}{r^2}-\frac{h^4}{r^4}+16\frac{h^4}{r^4}+8\frac{h^6}{r^6}-64\frac{h^6}{r^6}+\frac{h^8}{r^8}-48\frac{h^8}{r^8}+..\right)$$

$$= -\frac{2}{r^2}\frac{h^4}{r^4}\left(1-12\frac{h^4}{r^4}+12\frac{h^6}{r^6}+36\frac{h^8}{r^8}+\dots\right).\left(1+\frac{h^2}{r^2}+\frac{h^4}{r^4}+\frac{h^6}{r^6}+\frac{h^8}{r^8}+\dots\right).$$

$$\left(1+8\frac{h^2}{r^2}+51\frac{h^4}{r^4}+236\frac{h^6}{r^6}+1021\frac{h^8}{r^8}+\dots\right)$$

$$= -\frac{2}{r^2}\frac{h^4}{r^4}\left(1-12\frac{h^4}{r^4}+12\frac{h^6}{r^6}+36\frac{h^8}{r^8}+\dots\right).\left(1+9\frac{h^2}{r^2}+60\frac{h^4}{r^4}+296\frac{h^6}{r^6}+1317\frac{h^8}{r^8}+\dots\right).$$

So,

$$(38) \qquad B = -\frac{2}{r^2}\frac{h^4}{r^4}\left(1 + 9\frac{h^2}{r^2} + 48\frac{h^4}{r^4} + 200\frac{h^6}{r^6} + 705\frac{h^8}{r^8} + \dots\right).$$

Using (37) and (38), we get

$$(39) \qquad \|\hat{T}_n\|^2\Big|_{x=h} = \frac{r}{\pi}(A + B) = \frac{r}{\pi}\left(\frac{2h^8}{r^{10}} + 50\frac{h^{10}}{r^{12}} + 512\frac{h^{12}}{r^{14}} + \dots\right).$$

From (35), we get

$$\|T_n\|^2\Big|_{x=h} = \sum_{i=0}^{2}\alpha_i\left(\sum_{j=0}^{2}\alpha_j\frac{r}{2\pi[r^2-ijh^2]} + h^2\frac{ri^2h^2}{\pi[r^2-ih^2]^3}\right)$$

$$+ h^2\sum_{j=0}^{2}\alpha_j\frac{rj^2h^2}{\pi[r^2-jh^2]^3} + h^4\frac{2r}{\pi(r^2-h^2)^5}[r^2(r^2+4h^2)+h^4]$$

$$= \frac{r}{\pi}\Big[\ \sum_{i=0}^{2}\alpha_i\Big\{-\frac{1}{2r^2}+\frac{1}{(r^2-ih^2)}-\frac{1}{2(r^2-2ih^2)}\Big\}+2h^4\sum_{i=0}^{2}\alpha_i\frac{i^2}{[r^2-ih^2]^3}$$

$$+\ h^4\ \frac{2[r^2(r^2+4h^2)+h^4]}{(r^2-h^2)^5}\ \Big]$$

$$= \frac{r}{\pi}\ (A + C + D),\ \text{say},$$

where A is given by (37).

$$C = 2h^4\sum_{i=0}^{2}\alpha_i\frac{i^2}{[r^2-ih^2]^3} = 2h^4\Big[\frac{2}{[r^2-h^2]^3} - \frac{4}{[r^2-2h^2]^3}\Big]$$

$$= -\ \frac{4h^4(r^6-6r^2h^4+6h^6)}{(r^2-h^2)^3(r^2-2h^2)^3}$$

$$= -\ \frac{4}{r^2}\ \frac{h^4}{r^4}\Big(1-\frac{6h^4}{r^4}+\frac{6h^6}{r^6}\Big)\Big[1-\frac{h^2}{r^2}\Big]^{-3}\Big(1-\frac{2h^2}{r^2}\Big)^{-3}$$

$$= -\ \frac{4}{r^2}\ \frac{h^4}{r^4}\Big(1-\frac{6h^4}{r^4}+\frac{6h^6}{r^6}\Big)\cdot\Big(1+9\frac{h^2}{r^2}+48\frac{h^4}{r^4}+198\frac{h^6}{r^6}+684\frac{h^8}{r^8}\ +\ldots\Big),$$

so that

$$(40)\qquad C = -\ \frac{4}{r^2}\ \frac{h^4}{r^4}\Big(1+9\frac{h^2}{r^2}+42\frac{h^4}{r^4}+150\frac{h^6}{r^6}+450\frac{h^8}{r^8}\ +\ldots\Big).$$

$$D = h^4\ \frac{2[r^2(r^2+4h^2)+h^4]}{(r^2-h^2)^5} = \frac{2}{r^2}\ \frac{h^4}{r^4}\Big(1+\frac{4h^2}{r^2}+\frac{h^4}{r^4}\Big)\Big[1-\frac{h^2}{r^2}\Big]^{-5},$$

so that

$$(41)\qquad D = \frac{2}{r^2}\ \Big(\frac{h^4}{r^4}+9\frac{h^6}{r^6}+36\frac{h^8}{r^8}+100\frac{h^{10}}{r^{10}}+225\frac{h^{12}}{r^{12}}+\ldots\Big).$$

Using (37), (40) and (41) we get

$$(42)\qquad \|T_n\|^2\Big|_{x=h} = \frac{r}{\pi}\ (A+C+D) = \frac{r}{\pi}\ \Big(\frac{2h^8}{r^{10}}+50\frac{h^{10}}{r^{12}}+512\frac{h^{12}}{r^{14}}+\ldots\Big).$$

Comparing (39) and (42) we see, $\|\hat{T}_n\|^2\Big|_{x=h}$ and $\|T_n\|^2\Big|_{x=h}$ are equal

at least up to order of h^{12}.

(iii) <u>At a general point x:</u>

From (34),

$$\|\hat{T}_n\|^2\Big|_x = \frac{r}{\pi}(\hat{A}+\hat{B}), \quad \text{where } \hat{A} = \hat{A}_1+\hat{A}_2+\hat{A}_3, \text{ with}$$

$$\hat{A}_1 = \sum_{i=0}^{2}\alpha_i \frac{-1}{2(r^2-(x-h)(x-(1-i)h)}$$

$$= \frac{1}{2\{(r^2-x^2)+h(2x-h)\}} - \frac{1}{\{(r^2-x^2)+hx\}} + \frac{1}{2\{(r^2-x^2)+h^2\}},$$

$$\hat{A}_2 = \sum_{i=0}^{2}\alpha_i \frac{1}{(r^2-x(x-(1-i)h))}$$

$$= -\frac{1}{\{(r^2-x^2)+hx\}} + \frac{2}{(r^2-x^2)} - \frac{1}{\{(r^2-x^2)-hx\}},$$

$$\hat{A}_3 = \sum_{i=0}^{2}\alpha_i \frac{-1}{2(r^2-(x+h)(x-(1-i)h))}$$

$$= \frac{1}{2\{(r^2-x^2)+h^2\}} - \frac{1}{\{(r^2-x^2)-hx\}} + \frac{1}{2\{(r^2-x^2)-h(2x+h)\}},$$

so that

$$\hat{A} = \hat{A}_1+\hat{A}_2+\hat{A}_3 =$$

$$= \frac{2}{(r^2-x^2)} + \frac{1}{2\{(r^2-x^2)+h(2x-h)\}} + \frac{1}{2\{(r^2-x^2)-h(2x+h)\}} +$$

$$+ \frac{1}{\{(r^2-x^2)+h^2\}} - \frac{2}{\{(r^2-x^2)+hx\}} - \frac{2}{\{(r^2-x^2)-hx\}}$$

$$= \frac{2}{(r^2-x^2)} + \frac{1}{2(r^2-x^2)}\left[1+\frac{h(2x-h)}{(r^2-x^2)}\right]^{-1} + \frac{1}{2(r^2-x^2)}\left[1-\frac{h(2x+h)}{(r^2-x^2)}\right]^{-1} +$$

$$\frac{1}{(r^2-x^2)}\left[1+\frac{h^2}{r^2-x^2}\right]^{-1} - \frac{2}{(r^2-x^2)}\left[1+\frac{hx}{r^2-x^2}\right]^{-1} - \frac{2}{(r^2-x^2)}\left[1-\frac{hx}{r^2-x^2}\right]^{-1}.$$

Since the first term gets canceled and the last two terms get combined, we get

$$\hat{A} = \frac{1}{2(r^2-x^2)}\left[-\frac{h(2x-h)}{(r^2-x^2)}+\frac{h^2(2x-h)^2}{(r^2-x^2)^2}-\frac{h^3(2x-h)^3}{(r^2-x^2)^3}+\frac{h^4(2x-h)^4}{(r^2-x^2)^4}-\cdots\right]$$

$$+\frac{1}{2(r^2-x^2)}\left[\frac{h(2x+h)}{(r^2-x^2)}+\frac{h^2(2x+h)^2}{(r^2-x^2)^2}+\frac{h^3(2x+h)^3}{(r^2-x^2)^3}+\frac{h^4(2x+h)^4}{(r^2-x^2)^4}+\cdots\right]$$

$$+\frac{1}{(r^2-x^2)}\left[-\frac{h^2}{r^2-x^2}+\frac{h^4}{(r^2-x^2)^2}-\frac{h^6}{(r^2-x^2)^3}+\frac{h^8}{(r^2-x^2)^4}-\frac{h^{10}}{(r^2-x^2)^5}+\cdots\right]$$

$$-\frac{2}{(r^2-x^2)}\left[\frac{2h^2x^2}{(r^2-x^2)^2}+\frac{2h^4x^4}{(r^2-x^2)^4}+\frac{2h^6x^6}{(r^2-x^2)^6}+\frac{2h^8x^8}{(r^2-x^2)^8}+\frac{2h^{10}x^{10}}{(r^2-x^2)^{10}}+\cdots\right].$$

Using $(2x-h)^2 + (2x+h)^2 = 2(4x^2 + h^2)$,

$-(2x-h)^3 + (2x+h)^3 = 2(12x^2h + h^3)$,

$(2x-h)^4 + (2x+h)^4 = 2(16x^4 + 24x^2h^2 + h^4)$,

$-(2x-h)^5 + (2x+h)^5 = 2(80x^4h + 40x^2h^3 + h^5)$,

$(2x-h)^6 + (2x+h)^6 = 2(64x^6 + 240x^4h^2 + 60x^2h^4 + h^6)$,

$-(2x-h)^7 + (2x+h)^7 = 2(448x^6h + 560x^4h^3 + \cdots)$,

and $(2x-h)^8 + (2x+h)^8 = 2(256x^8 + 1792x^6h^2 + \cdots)$,

we get

$$(43)\qquad \hat{A} = = h^4\left\{\frac{2}{(r^2-x^2)^3}+\frac{12x^2}{(r^2-x^2)^4}+\frac{12x^4}{(r^2-x^2)^5}\right\}$$

$$+ h^6\left\{\frac{24x^2}{(r^2-x^2)^5}+\frac{80x^4}{(r^2-x^2)^6}+\frac{60x^6}{(r^2-x^2)^7}\right\}$$

$$+ h^8\left\{\frac{2}{(r^2-x^2)^5}+\frac{40x^2}{(r^2-x^2)^6}+\frac{240x^4}{(r^2-x^2)^7}+\frac{448x^6}{(r^2-x^2)^8}+\frac{252x^8}{(r^2-x^2)^9}\right\}+O(h^{10}).$$

$$\hat{B} = h^2\hat{\beta}_{1,n}\sum_{i=0}^{2}\alpha_i\frac{(x-(1-i)h)^2}{(r^2-x(x-(1-i)h))^3}$$

$$= h^2\hat{\beta}_{1,n}\left\{-\frac{(x-h)^2}{\{(r^2-x^2)+hx\}^3}+\frac{2x^2}{(r^2-x^2)^3}-\frac{(x+h)^2}{\{(r^2-x^2)-hx\}^3}\right\}$$

$$= h^2\hat{\beta}_{1,n}\left\{\frac{2x^2}{(r^2-x^2)^3}-\frac{(x-h)^2}{(r^2-x^2)^3}\left(1+\frac{hx}{r^2-x^2}\right)^{-3}-\frac{(x+h)^2}{(r^2-x^2)^3}\left(1-\frac{hx}{r^2-x^2}\right)^{-3}\right\}.$$

Using $(x-h)^2 + (x+h)^2 = 2(x^2+h^2)$ and substituting the value of $\hat{\beta}_{1,n}$, from (33), we get

$$\hat{B} = -h^4\left[1+\frac{(r^2-x^2)^2}{(r^4+4r^2x^2+x^4)}\left\{\frac{6x^2h^2}{(r^2-x^2)^2}+\frac{20x^4h^2}{(r^2-x^2)^3}+\frac{15x^6h^2}{(r^2-x^2)^4}+\frac{15x^4h^4}{(r^2-x^2)^4}\right.\right.$$

$$+\frac{42x^6h^4}{(r^2-x^2)^5}+\frac{28x^8h^4}{(r^2-x^2)^6}+\frac{28x^6h^6}{(r^2-x^2)^6}+\frac{72x^8h^6}{(r^2-x^2)^7}+\frac{45x^{10}h^6}{(r^2-x^2)^8}+\frac{45x^8h^8}{(r^2-x^2)^8}$$

$$\left.\left.+\frac{110x^{10}h^8}{(r^2-x^2)^9}+\frac{66x^{12}h^8}{(r^2-x^2)^{10}}+\cdots\cdots\right\}\right].$$

$$\cdot\left[\frac{2}{(r^2-x^2)^3}+\frac{12x^2}{(r^2-x^2)^4}+\frac{12x^4}{(r^2-x^2)^5}+\frac{12x^2h^2}{(r^2-x^2)^5}+\frac{40x^4h^2}{(r^2-x^2)^6}+\frac{30x^6h^2}{(r^2-x^2)^7}\right.$$

$$\left.+\frac{30x^4h^4}{(r^2-x^2)^7}+\frac{84x^6h^4}{(r^2-x^2)^8}+\frac{56x^8h^4}{(r^2-x^2)^9}+\frac{56x^6h^6}{(r^2-x^2)^9}+\frac{144x^8h^6}{(r^2-x^2)^{10}}+\frac{90x^{10}h^6}{(r^2-x^2)^{11}}+\cdots\cdots\right].$$

After simplifying, we get

$$(44)\qquad \hat{B} = -h^4\left[\frac{2}{(r^2-x^2)^3}+\frac{12x^2}{(r^2-x^2)^4}+\frac{12x^4}{(r^2-x^2)^5}\right]$$

$$-h^6\left[\frac{24x^2}{(r^2-x^2)^5}+\frac{80x^4}{(r^2-x^2)^6}+\frac{60x^6}{(r^2-x^2)^7}\right]-h^8\left[2\left\{\frac{30x^4}{(r^2-x^2)^7}+\frac{84x^6}{(r^2-x^2)^8}+\frac{56x^8}{(r^2-x^2)^9}\right\}\right.$$

$$\left.+\frac{2}{(r^2-x^2)(r^4+4r^2x^2+x^4)}\left\{\frac{6x^2}{(r^2-x^2)^2}+\frac{20x^4}{(r^2-x^2)^3}+\frac{15x^6}{(r^2-x^2)^4}\right\}^2\right]+O(h^{10}).$$

By (43) and (44), we get $\|\hat{T}_n\|^2 = \frac{r}{\pi}(\hat{A}+\hat{B})$, so that

$$(45) \qquad \|\hat{T}_n\|^2 = \frac{r}{\pi}h^8\Bigg[\frac{2}{(r^2-x^2)^5}+\frac{40x^2}{(r^2-x^2)^6}+\frac{180x^4}{(r^2-x^2)^7}+\frac{280x^6}{(r^2-x^2)^8}+\frac{140x^8}{(r^2-x^2)^9}$$

$$-\frac{2}{(r^2-x^2)(r^4+4r^2x^2+x^4)}\left(\frac{6x^2}{(r^2-x^2)^2}+\frac{20x^4}{(r^2-x^2)^3}+\frac{15x^6}{(r^2-x^2)^4}\right)^2\Bigg]+O(h^{10}).$$

Now by (35), $\|T_n\|^2 = \frac{r}{\pi}(\hat{A}+E+F)$, where $\hat{A}$ is given by (43). As

$$E = 2h^2\sum_{i=0}^{2}\alpha_i\frac{\{x-(1-i)h\}^2}{[r^2-\{x-(1-i)h\}x]^3},$$

$$= 2h^2\Bigg[\frac{2x^2}{(r^2-x^2)^3}-\frac{(x-h)^2}{(r^2-x^2)^3}\left(1+\frac{hx}{(r^2-x^2)}\right)^{-3}-\frac{(x+h)^2}{(r^2-x^2)^3}\left(1-\frac{hx}{(r^2-x^2)}\right)^{-3}\Bigg],$$

we have

$$(46) \qquad E = -2h^4\Bigg[\left(\frac{2}{(r^2-x^2)^3}+\frac{12x^2}{(r^2-x^2)^4}+\frac{12x^4}{(r^2-x^2)^5}\right)$$

$$+\left(\frac{12x^2h^2}{(r^2-x^2)^5}+\frac{40x^4h^2}{(r^2-x^2)^6}+\frac{30x^6h^2}{(r^2-x^2)^7}\right)+\left(\frac{30x^4h^4}{(r^2-x^2)^7}+\frac{84x^6h^4}{(r^2-x^2)^8}+\frac{56x^8h^4}{(r^2-x^2)^9}\right)$$

$$+\left(\frac{56x^6h^6}{(r^2-x^2)^9}+\frac{144x^8h^6}{(r^2-x^2)^{10}}+\frac{90x^{10}h^6}{(r^2-x^2)^{11}}\right)+\cdots\Bigg].$$

Also

$$(47) \qquad F = h^4\,\frac{2[r^2(r^2+4x^2)+x^4]}{(r^2-x^2)^5} = h^4\left[\frac{2}{(r^2-x^2)^3}+\frac{12x^2}{(r^2-x^2)^4}+\frac{12x^4}{(r^2-x^2)^5}\right].$$

Hence, by (43), (46) and (47), we get

$$(48) \qquad \|T_n\|^2 = \frac{r}{\pi}(\hat{A}+E+F)$$

$$= \frac{r}{\pi}h^8\left[\frac{2}{(r^2-x^2)^5}+\frac{40x^2}{(r^2-x^2)^6}+\frac{180x^4}{(r^2-x^2)^7}+\frac{280x^6}{(r^2-x^2)^8}+\frac{140x^8}{(r^2-x^2)^9}\right]+O(h^{10}).$$

Comparing (45) and (48), we get

$$\|T_n\|^2-\|\hat{T}_n\|^2 = \frac{r}{\pi}h^8\frac{2}{(r^2-x^2)(r^4+4r^2x^2+x^4)}\left(\frac{6x^2}{(r^2-x^2)^2}+\frac{20x^4}{(r^2-x^2)^3}+\frac{15x^6}{(r^2-x^2)^4}\right)^2\Bigg]+$$

$$+O(h^{10}).$$

So, we conclude that $\|T_n\|$, $\|\hat{T}_n\|$, $\|T_n\| - \|\hat{T}_n\|$ are of $O(h^4)$, for all $x \neq 0$, in $(-r,r)$.

Next let us consider Cowell's method with function evaluation at three points as the usual method, for solving numerically a differential equation (I), with some initial or boundary conditions, which is given by

$$\sum_{i=0}^{2} \alpha_i y_{n-1+i} + h^2 \sum_{i=0}^{2} \beta_i f_{n-1+i} = 0, \tag{49}$$

where $\alpha_0 = -1$, $\alpha_1 = 2$, $\alpha_2 = -1$; $\alpha_0 = 1/12$, $\alpha_1 = 10/12$, $\alpha_2 = 1/12$.

Let

$$\sum_{i=0}^{2} \alpha_i y_{n-1+i} + h^2 \sum_{i=0}^{2} \hat{\beta}_{i,n} f_{n-1+i} = 0 \tag{50}$$

be the corresponding β-optimal method, where $\hat{\beta}_{i,n}$ are the optimal coefficients at a point x_n, $1 \le n \le N-1$.

Now the local truncation error functional T_n at a point x_n of the usual method (49) applied to the true solution $y(x)$ is given by

$$T_n y = \sum_{i=0}^{2} \alpha_i y(x_{n-1+i}) + h^2 \sum_{i=0}^{2} \beta_i y''(x_{n-1+i}).$$

The representer for the local truncation error functional T_n is

$$\sum_{i=0}^{2} \bar{\alpha}_i K(t, \bar{x}_{n-1+i}) + h^2 \sum_{i=0}^{2} \bar{\beta}_i D2(t, \bar{x}_{n-1+i}), \text{ from which}$$

$$\|T_n\|^2 = \Big(\sum_{i=0}^{2} \bar{\alpha}_i K(t, \bar{x}_{n-1+i}) + h^2 \sum_{i=0}^{2} \bar{\beta}_i D2(t, \bar{x}_{n-1+i}),$$
$$\sum_{j=0}^{2} \bar{\alpha}_j K(t, \bar{x}_{n-1+j}) + h^2 \sum_{j=0}^{2} \bar{\beta}_j D2(t, \bar{x}_{n-1+j}) \Big),$$

is given by

$$(51)\quad \|T_n\|^2 = \sum_{i=0}^{2}\bar{\alpha}_i\left(\sum_{j=0}^{2}\alpha_j K(x_{n-1+j},\bar{x}_{n-1+i})+h^2\sum_{j=0}^{2}\beta_j \overline{D2(x_{n-1+i},\bar{x}_{n-1+j})}\right)$$

$$+\ h^2\sum_{i=0}^{2}\bar{\beta}_i\left(\sum_{j=0}^{2}\alpha_j D2(x_{n-1+j},\bar{x}_{n-1+i})+h^2\sum_{j=0}^{2}\beta_j D2''(x_{n-1+j},\bar{x}_{n-1+i})\right).$$

Using the normal equations for obtaining $\hat{\beta}_{j,n}$, $j = 0(1)2$, $\|\hat{T}_n\|^2$, the square norm of local truncation error functional of the β-optimal method is given by

$$(52)\quad \|\hat{T}_n\|^2 = \sum_{i=0}^{2}\bar{\alpha}_i\left(\sum_{j=0}^{2}\alpha_j K(x_{n-1+j},\bar{x}_{n-1+i})+h^2\sum_{j=0}^{2}\hat{\beta}_{j,n}\overline{D2(x_{n-1+i},\bar{x}_{n-1+j})}\right).$$

The normal equations for obtaining $\hat{\beta}_{i,n}$, $i = 0(1)2$ are given by

$$\sum_{i=0}^{2}\alpha_i D2(x_{n-1+i},\bar{x}_{n-1+k})+h^2\sum_{i=0}^{2}\hat{\beta}_{i,n}D2''(x_{n-1+i},\bar{x}_{n-1+k})=0,\quad k=0(1)2.$$

At $x = 0$, it gives the system of equations

$$D\beta = E,$$

where
$$D = -\,h^2\begin{bmatrix} D2''(-h,-h) & D2''(0,-h) & D2''(h,-h)\\ D2''(-h,0) & D2''(0,0) & D2''(h,0)\\ D2''(-h,h) & D2''(0,h) & D2''(h,h)\end{bmatrix},$$

$$\beta = \left[\ \hat{\beta}_{1,n},\ \hat{\beta}_{2,n},\ \hat{\beta}_{3,n}\ \right]^T,$$

$$E = \begin{bmatrix} -\ D2(-h,-h) & +\ 2D2(0,-h) & -\ D2(h,-h)\\ -\ D2(-h,0) & +\ 2D2(0,0) & -\ D2(h,0)\\ -\ D2(-h,h) & +\ 2D2(0,h) & -\ D2(h,h)\end{bmatrix}.$$

In $H^2(C_r)$-space, writing the values of D2 and D2″ at the nodal points, from (5) and (6), we get

$$D = \begin{bmatrix} a_1 & b_1 & c_1\\ b_1 & b_1 & b_1\\ c_1 & b_1 & a_1\end{bmatrix}\quad \text{and}\quad E = \begin{bmatrix} e_1\\ b_1\\ e_1\end{bmatrix},$$

with $a_1 = \dfrac{2r(r^4+4r^2h^2+h^4)}{(r^2-h^2)^5}$, $b_1 = \dfrac{2}{r^5}$, $c_1 = \dfrac{2r(r^4-4r^2h^2+h^4)}{(r^2+h^2)^5}$

and $e_1 = \dfrac{r}{(r^2-h^2)^3} + \dfrac{r}{(r^2+h^2)^3}$.

Solving the above system of equations we get the solution

$$\hat{\beta}_{1,n} = \frac{b_1 - e_1}{2b_1 - c_1 - a_1},\quad \hat{\beta}_{2,n} = \frac{2e_1 - c_1 - a_1}{2b_1 - c_1 - a_1},\quad \hat{\beta}_{3,n} = \frac{b_1 - e_1}{2b_1 - c_1 - a_1}.$$

Now, $b_1 - e_1 = \dfrac{2(r^4-h^4)^3 - r^6(r^2+h^2)^3 - r^6(r^2-h^2)^3}{r^5(r^4-h^4)^3}$,

$$2b_1-c_1-a_1 = \{4(r^4-h^4)^5-2r^6(r^2+h^2)^5(r^4+4r^2h^2+h^4) \\ -2r^6(r^2-h^2)^5(r^4-4r^2h^2+h^4)\}/r^5(r^4-h^4)^5,$$

$$2e_1-c_1-a_1 = \{[2r(r^2-h^2)^2(r^2+h^2)^5 + 2r(r^2+h^2)^2(r^2-h^2)^5 \\ -2r(r^2+h^2)^5(r^4+4r^2h^2+h^4)-2r(r^2-h^2)^5(r^4-4r^2h^2+h^4)]\}/(r^4-h^4)^5$$

$$\hat{\beta}_{1,n} = \hat{\beta}_{3,n} = \text{Num1}/\text{Din1} =$$

$$= \frac{2(r^4-h^4)^5 - r^6(r^2+h^2)^3(r^4-h^4)^2 - r^6(r^2-h^2)^3(r^4-h^4)^2}{4(r^4-h^4)^5 - 2r^6(r^2+h^2)^5(r^4+4r^2h^2+h^4) - 2r^6(r^2-h^2)^5(r^4-4r^2h^2+h^4)}.$$

$$\begin{aligned}\text{Din1} &= \left\{2(r^4-h^4)^5 - 2r^6(r^2+h^2)^5(r^4+4r^2h^2+h^4)\right\} \\ &\quad + \left\{2(r^4-h^4)^5 - 2r^6(r^2-h^2)^5(r^4-4r^2h^2+h^4)\right\} \\ &= 2(r^2+h^2)^5\left\{-9r^8h^2 + 9r^6h^4 - 10r^4h^6 + 5r^2h^8 - h^{10}\right\} \\ &\quad + 2(r^2-h^2)^5\left\{9r^8h^2 + 9r^6h^4 + 10r^4h^6 + 5r^2h^8 + h^{10}\right\}.\end{aligned}$$

Using $(r^2+h^2)^5 + (r^2-h^2)^5 = 2(r^{10} + 10r^6h^4 + 5r^2h^8)$

and $-(r^2+h^2)^5 + (r^2-h^2)^5 = -2(5r^8h^2 + 10r^4h^6 + h^{10})$, we get

$$\begin{aligned}\text{Din1} &= -36r^8h^2(5r^8h^2+10r^4h^6+h^{10})+36r^6h^4(r^{10}+10r^6h^4+5r^2h^8) \\ &\quad - 40r^4h^6(5r^8h^2+10r^4h^6+h^{10})+20r^2h^8(r^{10}+10r^6h^4+5r^2h^8)\end{aligned}$$

$$- 4h^{10}(5r^8h^2 + 10r^4h^6 + h^{10})$$

$$= - 144r^{16}h^4-180r^{12}h^8-76r^8h^{12}+20r^4h^{16}-4h^{20}, \text{ and}$$

$$\text{Num1} = 2(r^4-h^4)^5-r^6(r^4-h^4)^2\left\{(r^2+h^2)^3+(r^2-h^2)^3\right\}$$

$$= 2(r^{20}-5r^{16}h^4+10r^{12}h^8-10r^8h^{12}+5r^4h^{16}-h^{20})$$

$$-r^6(r^8-2r^4h^4+h^8)(2r^6+6r^2h^4)$$

$$= - 12r^{16}h^4+30r^{12}h^8- 26r^8h^{12} + 10r^4h^{16} - 2h^{20}. \text{ Hence}$$

$$\hat{\beta}_{1,n} = \hat{\beta}_{3,n} = \frac{- 12r^{16}h^4 + 30r^{12}h^8 - 26r^8h^{12} + 10r^4h^{16} - 2h^{20}}{- 144r^{16}h^4 - 180r^{12}h^8 - 76r^8h^{12} + 20r^4h^{16} - 4h^{20}}$$

$$=\frac{1}{144}\left(12-30\frac{h^4}{r^4}+26\frac{h^8}{r^8}-10\frac{h^{12}}{r^{12}}+2\frac{h^{16}}{r^{16}}\right)\left(1+\frac{180}{144}\frac{h^4}{r^4}+\frac{76}{144}\frac{h^8}{r^8}-\frac{20}{144}\frac{h^{12}}{r^{12}}+\frac{4}{144}\frac{h^{16}}{r^{16}}\right)^{-1}$$

$$= \left(\frac{1}{12}-\frac{5}{24}\frac{h^4}{r^4}+\frac{13}{72}\frac{h^8}{r^8}-\frac{5}{72}\frac{h^{12}}{r^{12}}+\frac{1}{72}\frac{h^{16}}{r^{16}}\right)\left[1+\left\{\frac{5}{4}\frac{h^4}{r^4}+\frac{19}{36}\frac{h^8}{r^8}-\frac{5}{36}\frac{h^{12}}{r^{12}}+\frac{1}{36}\frac{h^{16}}{r^{16}}\right\}\right]^{-1}$$

$$= \left(\frac{1}{12}-\frac{5}{24}\frac{h^4}{r^4}+\frac{13}{72}\frac{h^8}{r^8}-\frac{5}{72}\frac{h^{12}}{r^{12}}+\frac{1}{72}\frac{h^{16}}{r^{16}}\right)\left[1-\left\{\frac{5}{4}\frac{h^4}{r^4}+\frac{19}{36}\frac{h^8}{r^8}-\frac{5}{36}\frac{h^{12}}{r^{12}}+\frac{1}{36}\frac{h^{16}}{r^{16}}\right\}\right.$$

$$\left.+\left\{\frac{5}{4}\frac{h^4}{r^4}+\frac{19}{36}\frac{h^8}{r^8}-\frac{5}{36}\frac{h^{12}}{r^{12}}+\frac{1}{36}\frac{h^{16}}{r^{16}}\right\}^2 + \left\{\frac{5}{4}\frac{h^4}{r^4}+\frac{19}{36}\frac{h^8}{r^8}-\frac{5}{36}\frac{h^{12}}{r^{12}}+\frac{1}{36}\frac{h^{16}}{r^{16}}\right\}^3+\ldots\right]$$

$$(53) \quad \hat{\beta}_{1,n} = \hat{\beta}_{3,n} = \frac{1}{12} - \frac{5}{16}\frac{h^4}{r^4}+\frac{911}{1728} - \frac{h^8}{r^8} - \frac{3815}{6912}\frac{h^{12}}{r^{12}} +\ldots$$

$$\hat{\beta}_{2,n} = \frac{\text{Num2}}{\text{Din2}} = (2r^6(r^2-h^2)^2(r^2+h^2)^5 + 2r^6(r^2+h^2)^2(r^2-h^2)^5 - $$
$$- 2r^6(r^2+h^2)^5(r^4+4r^2h^2+h^4) - 2r^6(r^2-h^2)^5(r^4-4r^2h^2+h^4))/$$
$$(4(r^4-h^4)^5-2r^6(r^2+h^2)^5(r^4+4r^2h^2+h^4)-2r^6(r^2-h^2)^5(r^4-4r^2h^2+h^4))$$

$$\text{Num2} = 2r^6(r^2+h^2)^5\left((r^2-h^2)^2- (r^4+4r^2h^2+h^4)\right)$$

$$+ 2r^6(r^2-h^2)^5\left((r^2+h^2)^2 - (r^4-4r^2h^2+h^4)\right)$$

$$= 12\left(- 10r^{16}h^4 - 20r^{12}h^8 - 2r^8h^{12}\right).$$

$$\mathrm{Din2} = \mathrm{Din1} = -144r^{16}h^4-180r^{12}h^8-76r^8h^{12}+20r^4h^{16}-4h^{20}.$$

So, $$\hat{\beta}_{2,n} = \frac{12}{144}\left(10+20\frac{h^4}{r^4}+2\frac{h^8}{r^8}\right)\left[1+\left\{\frac{5}{4}\,\frac{h^4}{r^4}+\frac{19}{36}\,\frac{h^8}{r^8}-\frac{5}{36}\,\frac{h^{12}}{r^{12}}+\frac{1}{36}\,\frac{h^{16}}{r^{16}}\right\}\right]^{-1}$$

$$= \frac{1}{12}\left(10+20\frac{h^4}{r^4}+2\frac{h^8}{r^8}\right)\times$$

$$\times\left[1-\left\{\frac{5}{4}\,\frac{h^4}{r^4}+\frac{19}{36}\,\frac{h^8}{r^8}-\frac{5}{36}\,\frac{h^{12}}{r^{12}}+\frac{1}{36}\,\frac{h^{16}}{r^{16}}\right\}+\left\{\frac{5}{4}\,\frac{h^4}{r^4}+\frac{19}{36}\,\frac{h^8}{r^8}-\frac{5}{36}\,\frac{h^{12}}{r^{12}}+\frac{1}{36}\,\frac{h^{16}}{r^{16}}\right\}^2+\dots\right],$$

so that

$$(54)\quad \hat{\beta}_{2,n} = \frac{1}{12}\left(10+\frac{15}{2}\,\frac{h^4}{r^4}-\frac{911}{72}\,\frac{h^8}{r^8}+\frac{7365}{288}\,\frac{h^{12}}{r^{12}}+\dots\right).$$

For the usual method (49), from (51) we get

$$\|T_n\|^2\Big|_{x=0} = \frac{r}{\pi}\left[\sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\alpha_j\,\frac{1}{2[r^2-(j-1)(i-1)h^2]}+\right.$$

$$2h^4\sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\beta_j\,\frac{(i-1)^2}{[r^2-(j-1)(i-1)h^2]^3}+$$

$$\left.h^4\sum_{i=0}^{2}\beta_i\sum_{j=0}^{2}\beta_j\,\frac{2[r^2\{r^2+4(i-1)(j-1)h^2\}+(i-1)^2(j-1)^2h^4]}{[r^2-(j-1)(i-1)h^2]^5}\right]$$

$$= \frac{r}{\pi}\,(X+Y+Z),\ \text{say}.$$

For the optimal method (50), from (52) we get

$$\|\hat{T}_n\|^2\Big|_{x=0} = \frac{r}{\pi}\left[\sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\alpha_j\,\frac{1}{2[r^2-(j-1)(i-1)h^2]}+\right.$$

$$\left.h^4\sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\hat{\beta}_{j,n}\,\frac{(i-1)^2}{[r^2-(j-1)(i-1)h^2]^3}\right]$$

$$= \frac{r}{\pi}\,(X+W),\ \text{say}.$$

Hence, $$\|T_n\|^2\Big|_{x=0} - \|\hat{T}_n\|^2\Big|_{x=0} = \frac{r}{\pi}\,(Y+Z-W).$$

Now, $$X = \sum_{i=0}^{2} \alpha_i \sum_{j=0}^{2} \alpha_j \frac{1}{2[r^2-(j-1)(i-1)h^2]}$$

$$= \sum_{i=0}^{2} \alpha_i \left[\frac{-1}{2[r^2+(i-1)h^2]}+\frac{1}{r^2}+\frac{-1}{2[r^2-(i-1)h^2]}\right]$$

$$= \frac{1}{r^2-h^2}-\frac{2}{r^2}+\frac{1}{r^2+h^2} = \frac{1}{r^2}\left(1-\frac{h^2}{r^2}\right)^{-1}+\frac{1}{r^2}\left(1+\frac{h^2}{r^2}\right)^{-1}-\frac{2}{r^2},$$

so that

$$X = 2\frac{h^4}{r^6}+2\frac{h^8}{r^{10}}+2\frac{h^{12}}{r^{14}}+2\frac{h^{16}}{r^{18}}+\ldots\ldots\ . \tag{55}$$

$$Y = 2h^4 \sum_{i=0}^{2} \alpha_i \sum_{j=0}^{2} \beta_j \frac{(i-1)^2}{[r^2-(j-1)(i-1)h^2]^3}$$

$$= 2h^4 \sum_{i=0}^{2} \alpha_i (i-1)^2 \left\{\frac{\beta_0}{[r^2+(i-1)h^2]^3}+\frac{\beta_1}{(r^2)^3}+\frac{\beta_2}{[r^2-(i-1)h^2]^3}\right\}$$

$$= 2h^4\left[\alpha_1\left\{\frac{1}{12}\ \frac{1}{[r^2-h^2]^3}+\frac{10}{12}\ \frac{1}{r^6}+\frac{1}{12}\ \frac{1}{[r^2+h^2]^3}\right\}\right.$$

$$\left. + \ \alpha_3\left\{\frac{1}{12}\ \frac{1}{[r^2+h^2]^3}+\frac{10}{12}\ \frac{1}{r^6}+\frac{1}{12}\ \frac{1}{[r^2-h^2]^3}\right\}\right]$$

$$= -\ 2h^4\left[\frac{5}{3}\ \frac{1}{r^6}+\frac{1}{6}\ \frac{1}{r^6}\left(1-\frac{h^2}{r^2}\right)^{-3}+\frac{1}{6}\ \frac{1}{r^6}\left(1+\frac{h^2}{r^2}\right)^{-3}\right]$$

$$= -\ 2h^4\left[\frac{5}{3}\ \frac{1}{r^6}+\frac{1}{6}\ \frac{1}{r^6}\left(2+12\frac{h^4}{r^4}+30\frac{h^6}{r^6}+56\frac{h^8}{r^8}+\ldots\ldots\right)\right],$$ so that

$$Y = -\ 4\frac{h^4}{r^6}-4\frac{h^8}{r^{10}}-10\frac{h^{12}}{r^{14}}-\frac{56}{3}\ \frac{h^{16}}{r^{18}}+\ldots\ldots\ . \tag{56}$$

$$Z = h^4 \sum_{i=0}^{2} \beta_i \sum_{j=0}^{2} \beta_j \frac{2[r^2(r^2+4(i-1)(j-1)h^2) \ + \ (i-1)^2(j-1)^2h^4]}{[r^2-(j-1)(i-1)h^2]^5}$$

$$= \ 2h^4 \sum_{i=0}^{2} \beta_i \left\{\beta_0 \frac{[r^2(r^2-4(i-1)h^2)+(i-1)^2h^4]}{[r^2+(i-1)h^2]^5} \ + \ \beta_1\ \frac{1}{r^6} \ + \right.$$

$$+\beta_2\frac{[r^2\{r^2+4(i-1)h^2\}+(i-1)^2h^4]}{[r^2-(i-1)h^2]^5}\Bigg\}$$

$$= 2h^4\left[\beta_0\left\{\beta_0\frac{r^2(r^2+4h^2)+h^4}{[r^2-h^2]^5}+\beta_1\frac{1}{r^6}+\beta_2\frac{r^2(r^2-4h^2)+h^4}{[r^2+h^2]^5}\right\}+\beta_1\frac{1}{r^6}\sum_{i=0}^{2}\beta_i+\right.$$

$$\left.\beta_2\left\{\beta_0\frac{r^2(r^2-4h^2)+h^4}{[r^2+h^2]^5}+\beta_1\frac{1}{r^6}+\beta_2\frac{r^2(r^2+4h^2)+h^4}{[r^2-h^2]^5}\right\}\right].$$

Using the fact that $\beta_0 = \beta_2$, and $\sum_{i=0}^{2}\beta_i = 1$,

$$Z = 2h^4\left[2\beta_0\left\{\beta_0\frac{r^2(r^2+4h^2)+h^4}{[r^2-h^2]^5}+\beta_1\frac{1}{r^6}+\beta_2\frac{r^2(r^2-4h^2)+h^4}{[r^2+h^2]^5}\right\}+\beta_1\frac{1}{r^6}\right]$$

$$= 2\frac{h^4}{r^6}\left[\beta_1+2\beta_0\left\{\beta_0\left(1+4\frac{h^2}{r^2}+\frac{h^4}{r^4}\right)\left(1-\frac{h^2}{r^2}\right)^{-5}+\beta_0\left(1-4\frac{h^2}{r^2}+\frac{h^4}{r^4}\right)\left(1+\frac{h^2}{r^2}\right)^{-5}+\beta_1\right\}\right].$$

Using $\left(1-\frac{h^2}{r^2}\right)^{-5}+\left(1+\frac{h^2}{r^2}\right)^{-5} = 2\left(1+15\frac{h^4}{r^4}+70\frac{h^8}{r^8}+210\frac{h^{12}}{r^{12}}+\ldots\ldots\right)$

and $\left(1-\frac{h^2}{r^2}\right)^{-5} - \left(1+\frac{h^2}{r^2}\right)^{-5} = 2\left(5\frac{h^2}{r^2}+35\frac{h^6}{r^6}+126\frac{h^{10}}{r^{10}}+\ldots\ldots\right)$, we get

$$(57)\qquad Z = 2\frac{h^4}{r^6}\left[\beta_1+2\beta_0\left\{(\beta_1+2\beta_0)+\frac{h^4}{r^4}72\beta_0+450\beta_0\frac{h^8}{r^8}+1568\beta_0\frac{h^{12}}{r^{12}}+\ldots.\right\}\right].$$

Substituting the values of β_0 and β_1, we get

$$Z = 2\frac{h^4}{r^6}+2\frac{h^8}{r^{10}}+\frac{25}{2}\frac{h^{12}}{r^{14}}+\frac{98.4}{9}\frac{h^{16}}{r^{18}}+\ldots\ldots .$$

$$W = h^4\sum_{i=0}^{2}\alpha_i\sum_{j=0}^{2}\hat{\beta}_{j,n}\frac{(i-1)^2}{[r^2-(j-1)(i-1)h^2]^3}$$

$$= h^4\sum_{i=0}^{2}\alpha_i(i-1)^2\left\{\frac{\hat{\beta}_{0,n}}{[r^2+(i-1)h^2]^3}+\frac{\hat{\beta}_{1,n}}{(r^2)^3}+\frac{\hat{\beta}_{2,n}}{[r^2-(i-1)h^2]^3}\right\}$$

$$=h^4\left[\hat{\beta}_{0,n}\left\{\frac{\alpha_1}{[r^2-h^2]^3}+\frac{\alpha_3}{[r^2+h^2]^3}\right\}+\hat{\beta}_{1,n}\frac{\alpha_1+\alpha_3}{r^6}+\hat{\beta}_{2,n}\left\{\frac{\alpha_1}{[r^2+h^2]^3}+\frac{\alpha_3}{[r^2-h^2]^3}\right\}\right].$$

Since $\hat{\beta}_{0,n} = \hat{\beta}_{2,n}$ and $\alpha_1 = \alpha_3 = -1$, we get

$$W = -h^4\left[2\hat{\beta}_{0,n}\left\{\frac{1}{[r^2-h^2]^3}+\frac{1}{[r^2+h^2]^3}\right\}+2\hat{\beta}_{1,n}\frac{1}{r^6}\right]$$

$$= -2\frac{h^4}{r^6}\left[\hat{\beta}_{0,n}\left\{\left(1-\frac{h^2}{r^2}\right)^{-3}+\left(1+\frac{h^2}{r^2}\right)^{-3}\right\}+\hat{\beta}_{1,n}\right]$$

$$= -2\frac{h^4}{r^6}\left[2\hat{\beta}_{0,n}\left(1+6\frac{h^4}{r^4}+15\frac{h^8}{r^8}+28\frac{h^{12}}{r^{12}}+\dots\dots\right)+\hat{\beta}_{1,n}\right]$$

$$W = -2\frac{h^4}{r^6}\left[2\left\{\left(\frac{1}{12}-\frac{5}{16}\frac{h^4}{r^4}+\frac{911}{1728}\frac{h^8}{r^8}-\frac{3815}{6912}\frac{h^{12}}{r^{12}}+\dots\right)\left(1+6\frac{h^4}{r^4}+15\frac{h^8}{r^8}+28\frac{h^{12}}{r^{12}}+\dots\right)\right.\right.$$

$$\left.\left.+\left(\frac{10}{12}+\frac{15}{24}\frac{h^4}{r^4}-\frac{911}{864}\frac{h^8}{r^8}+\frac{7365}{288}\frac{h^{12}}{r^{12}}+\dots\right)\right]\right], \text{ [by (53) and (54)]}$$

$$= -2\frac{h^4}{r^6}\left[\left(\frac{1}{6}+\frac{3}{8}\frac{h^4}{r^4}-\frac{169}{864}\frac{h^8}{r^8}+\frac{3512}{6912}\frac{h^{12}}{r^{12}}+\dots\right)\right.$$

$$\left.+\left(\frac{5}{6}+\frac{5}{8}\frac{h^4}{r^4}-\frac{911}{864}\frac{h^8}{r^8}+\frac{7365}{288}\frac{h^{12}}{r^{12}}+\dots\right)\right], \text{ so that}$$

(58) $$W = -2\frac{h^4}{r^6}-2\frac{h^8}{r^{10}}+\frac{5}{2}\frac{h^{12}}{r^{14}}-\frac{180314}{6912}\frac{h^{16}}{r^{18}}+\dots$$

By (56), (57), (58) we get

$$\|T_n\|^2\Big|_{x=0} - \|\hat{T}_n\|^2\Big|_{x=0} = \frac{r}{\pi}(Y+Z-W) = \frac{r}{\pi}\left[\frac{180314}{6912}\frac{h^{16}}{r^{18}}+O(h^{16})\right].$$

Thus we conclude that at $x = 0$, $\|T_n\| - \|\hat{T}_n\|$ is of $O(h^8)$.

Because of the complexity of calculation, we are omitting the similar evaluations for the methods (49) and (50) at x=h, and at a general point x. Similar results could also be obtained for other optimal methods discussed in Chapter 1.

CHAPTER - 5

OPTIMAL MULTISTEP METHODS IN $L^2(\hat{C}_r)$ SPACE

5.1 Introduction

Similar to $H^2(C_r)$ space, in $L^2(\hat{C}_r)$ space the norm is based on area integral on the disk D_r and so the points inside C_r get more weightage than the points on the boundary of C_r. Consequently the optimal multistep methods obtained in $L^2(\hat{C}_r)$ space are expected to result in a better distributed behavior in the central region of a subinterval [a,b] of (-r,r). In set theoretic notation, we note that

$$L^2(\hat{C}_r) \supset H^2(C_r).$$

In this chapter we study the optimal multistep methods discussed in Chapter 1 for the Hilbert space $L^2(\hat{C}_r)$. For the purpose of numerical illustration, as usual methods, we have taken Stormer's method with function evaluation at one point and Cowell's method with function evaluation at three points for boundary value problems and Cowell's method with function evaluation at three points and Stormer's method with function evaluation at five points for initial value problems. The interpolatory functions tell that the optimal methods admit functions of higher growth in $L^2(\hat{C}_r)$ space than in $H^2(C_r)$ space.

In section 5.2, we prove that the second derivative of the kernel function of $L^2(\hat{C}_r)$ space is the complex conjugate of the representer for the second derivative evaluation functional in $L^2(\hat{C}_r)$ space. We devote section 4.3 to the discussion of optimal

multistep methods in $L^2(\hat{C}_r)$ space and their numerical implementation, section 4.4 to the discussion of optimal multistep methods interpolatory for polynomials of certain degree and their numerical illustrations and section 4.5 to the discussion of optimal multistep methods interpolatory for linearly independent functions and their numerical illustrations. In section 4.6, we describe the limiting behavior of the optimal coefficients in the optimal methods in $L^2(\hat{C}_r)$ space as $r \to \infty$.

5.2 The Hilbert space $L^2(\hat{C}_r)$

The space $L^2(D_r)$ consists of measurable functions of complex variable z defined on the disc $D_r = \{z : |z| < r\}$ which are square integrable in D_r. The space $L^2(D_r)$ turns out to be a complex Hilbert space, with the inner product

$$(h,k) = \iint_{D_r} h(z)\, \overline{k(z)}\, dxdy, \qquad h,k \in L^2(D_r).$$

The subspace of $L^2(D_r)$, consisting of functions of complex variable z $(z = x + iy)$ which are analytic within the disc $D_r = \{z : |z| < r\}$, is a closed subspace and has infinite dimension. This subspace turns out to be a complex Hilbert space $L^2(\hat{C}_r)$ with the induced inner product given by

(1) $$(f,g) = \iint_{D_r} f(z)\, \overline{g(z)}\, dxdy, \qquad f,g \in L^2(C_r).$$

The space $L^2(\hat{C}_r)$ possesses a reproducing kernel function given by

(2) $$K(z,\bar{t}) = \frac{r^2}{\pi(r^2 - z\bar{t})^2},$$

and is separable with a complete orthonormal sequence $\{\psi_k\}$ of functions given by

(3) $$\psi_k(z) = \frac{z^k}{\sqrt{\pi}\; r^{k+1}}, \qquad k = 0,1,2.....$$

As the space $L^2(\hat{C}_r)$ possesses a reproducing kernel function, the linear functional for point evaluation:

$$L_z : f \longrightarrow f(z), \qquad f \in L^2(\hat{C}_r),\ z \in D_r$$

is a bounded linear functional (Aronszajn [4]).

Also the linear functional for k-th derivative evaluation

$$Dk_z : f \longrightarrow f^k(z), \qquad f \in L^2(\hat{C}_r),\ z \in D_r,$$

where k is a positive integer, is a bounded linear functional (Brij Bhusan [27]):

Theorem 1 : For $z \in D_r$ and k any positive integer Dk_z is a bounded linear functional in $L^2(\hat{C}_r)$ with

$$\| Dk_z \| \le k! \sqrt{\frac{r}{2\pi}} \left(\frac{2}{r-|z|} \right)^{k+\frac{3}{2}} .$$

Now we shall show that the complex conjugate of the second derivative of the kernel is the representer for the second derivative evaluation functional in $L^2(\hat{C}_r)$ space. We have

$$\overline{\frac{\partial^2}{\partial z^2} K(z,\bar{t})}\Big|_{z=z_0} = \frac{6r^2t^2}{\pi(r^2-\bar{z}_0t)^4}.$$

Theorem 2: The function

$$D2(t,\bar{z}_0) = \frac{6r^2t^2}{\pi(r^2-\bar{z}_0t)^4}$$

is the representer for the 2-nd derivative evaluation functional at $z_0 \in D_r$.

Proof: The only singularity of $D2(t,\bar{z}_0)$ is a pole of order 4 at $t = \frac{r^2}{\bar{z}_0}$. As $z_0 \varepsilon D_r$, $\frac{r^2}{\bar{z}_0}$ lies outside $C_r = \{z : |z| = r\}$. Hence the function $D2(t,\bar{z}_0)$ is analytic inside D_r and hence it belongs to $L^2(\hat{C}_r)$. We have to show that

$$f''(z_0) = \left(f(t) \;,\; \frac{6r^2t^2}{\pi(r^2-\bar{z}_0 t)^4}\right).$$

Now,
$$\left(f(t) \;,\; \frac{6r^2t^2}{\pi(r^2-\bar{z}_0t)^4}\right) = \iint_{D_r} f(t)\, \frac{6r^2\bar{t}^2}{\pi(r^2-z_0\bar{t})^4}\, dxdy$$

$$= \int_{\rho=0}^{r}\int_{\theta=0}^{2\pi} f(\rho e^{i\theta})\, \frac{6r^2\rho^2e^{-2i\theta}}{\pi(r^2-z_0\rho e^{-i\theta})^4}\, \rho d\theta d\rho, \qquad (\text{putting } t = \rho e^{i\theta})$$

$$= \int_{\rho=0}^{r}\left\{\int_{\theta=0}^{2\pi} f(\rho e^{i\theta})\, \frac{6r^2}{\pi\left(\frac{r^2}{\rho^2}\,\rho e^{i\theta} - z_0\right)^4}\, \frac{(\rho e^{i\theta})^2}{\rho^4}\, \frac{\rho i e^{i\theta} d\theta}{i e^{i\theta}}\right\} d\rho$$

$$= \int_{\rho=0}^{r}\left\{\int_{C_r} f(t)\, \frac{1}{\pi i}\, \frac{6r^2}{\left(t - z_0\frac{\rho^2}{r^2}\right)^4}\, \frac{t^2}{\rho^3}\left(\frac{\rho^2}{r^2}\right)^4 \frac{1}{t}\, dt\right\} d\rho$$

$$= \int_{\rho=0}^{r} \frac{6\rho^5}{r^6}\left\{\int_{C_r} \frac{1}{\pi i}\, \frac{f(t)t}{\left(t - z_0\frac{\rho^2}{r^2}\right)^4}\, dt\right\} d\rho$$

$$= \int_{\rho=0}^{r} \frac{2\rho^5}{r^6}\left\{\frac{3!}{2\pi i}\int_{C_r} \frac{f(t)t}{(t - t_0)^4}\, dt \Bigg|_{t_0 = z_0\frac{\rho^2}{r^2}}\right\} d\rho.$$

By using Cauchy integral formula for third derivative, we get

$$\left(f(t) \;,\; \frac{6r^2t^2}{\pi(r^2-\bar{z}_0t)^4}\right) = \int_{\rho=0}^{r} \frac{2\rho^5}{r^6}\, [f(z)z]^{(3)}\Big|_{z=z_0\frac{\rho^2}{r^2}}\, d\rho$$

$$= \int_{\rho=0}^{r} \frac{2\rho^5}{r^6} \left[zf^{(3)}(z) + 3f''(z)\right]\Big|_{z=z_0\frac{\rho^2}{r^2}} \, d\rho.$$

If $z_0 = 0$, the last integral equals to

$$\int_{\rho=0}^{r} \frac{2\rho^5}{r^6} [0.f^{(3)}(0) + 3f''(0)]d\rho = 3f''(0) \int_{\rho=0}^{r} \frac{2\rho^5}{r^6} d\rho = f''(0).$$

On the other hand, if $z_0 \neq 0$, the last integral equals

$$\int_{\rho=0}^{r} [f(z)z]^{(3)}\Big|_{z=z_0\frac{\rho^2}{r^2}} \frac{\rho^4}{z_0 r^4} \frac{2\rho}{r^2} z_0 \, d\rho$$

$$= \int_{z=0}^{z_0} [f(z)z]^{(3)} \frac{1}{z_0} \frac{z^2}{z_0^2} \, dz \quad = \frac{1}{z_0^3} \int_{z=0}^{z_0} [f(z)z]^{(3)} z^2 \, dz$$

$$= \frac{1}{z_0^3}\left[[f(z)z]'' z^2\Big|_{z=0}^{z_0} - \int_{z=0}^{z_0} [f(z)z]''2zdz\right] \text{ (Integrating by parts)}$$

$$= \frac{1}{z_0^3} \left[\left([f(z)z]'' z^2\right)\Big|_{z=0}^{z_0} - \left([f(z)z]' \; 2z\right)\Big|_{z=0}^{z_0} + \left(2[f(z)z]\right)\Big|_{z=0}^{z_0}\right]$$

$$= \frac{1}{z_0^3} \left[\left(f''(z_0)z_0+2f'(z_0)\right)z_0^2 - \left(f'(z_0)z_0+f(z_0)\right)2z_0+2f(z_0)z_0\right]$$

$= f''(z_0)$. Hence the proof.

In $L^2(\hat{C}_r)$ space, we have the following formulae:

(4) $$K(z,\bar{t}) = \frac{r^2}{\pi(r^2-z\bar{t})^2},$$

(5) $$D2(t,\bar{z}) = \overline{\frac{\partial^2}{\partial z^2} K(z,\bar{t})} = \frac{6r^2}{\pi} \frac{t^2}{(r^2-t\bar{z})^4},$$

(6) $$D2''(t,\bar{z}) = \frac{\partial^2}{\partial t^2} D2(t,\bar{z}) = \frac{12r^2}{\pi} \frac{1}{(r^2-t\bar{z})^4}\left[1 + \frac{8t\bar{z}}{(r^2-t\bar{z})} + \frac{10t^2\bar{z}^2}{(r^2-t\bar{z})^2}\right].$$

As in $H^2(C_r)$ space, in $L^2(\hat{C}_r)$ space we shall implement some optimal multistep methods discussed in Chapter 1, especially (i) β-optimal methods (ii) α-optimal methods, (iii) β-optimal methods with restriction (10) in the sequel, (iv) β-optimal methods interpolatory for polynomials of certain degree, and (v) β-optimal methods interpolatory for certain linearly independent functions corresponding to Cowell's usual method with function evaluation at three points, for the 24 BVP-s and 24 IVP-s with differential equations and solutions 1-24 listed in Chapter 4. We also implement β- optimal methods corresponding to Stormer's usual explicit method with function evaluation at five points on the same 24 IVP's and β-optimal methods corresponding to Stormer's usual method with function evaluation at one point for the same 24 BVP's. As the solutions of these 24 equations have singularities of different kinds at various locations, they require, for various ranges of intervals, different domains of space $L^2(\hat{C}_r)$ for showing better performance of several optimal methods than the corresponding usual method. The solutions of the equations 1-9 and 19-24 are having singularities near the boundary of the domain of $L^2(\hat{C}_r)$ space with r=2.01. The solutions of the equations 10-12 are entire functions and the solutions of the equations 13-18 are having singularities far from the boundary of the domain of $L^2(\hat{C}_r)$ space with r = 2.01. The optimal methods are performing worse than the corresponding usual methods for the equations 10-18 with r=2.01. However with larger values of r and with larger intervals, optimal methods

perform better than the corresponding usual methods for the equations 10-18. The key symbols used in the tables of this chapter are the same as given in Chapter 4.

5.3 Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space

In $L^2(\hat{C}_r)$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$, of the β-optimal multistep method

$$(7) \qquad \sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} f_{n+k-j} = 0,$$

where α_j' s are prefixed according to some consistent and stable known usual method with highest degree polynomial precision

$$(8) \qquad \sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0,$$

with reference to equation (11) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where

$$\hat{b} = h^2\left(\hat{\beta}_{\delta_{t0},n},\ldots\ldots\ldots,\hat{\beta}_{k,n}\right)^T,$$

$$\hat{c}_{ij} = \frac{12r^2}{\pi}\frac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4}\left[1 + \frac{8x_{n+k-j}\bar{x}_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})} + \frac{10x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}\right],$$

$$i,j = \delta_{t0}(1)k,$$

and

$$\hat{d}_i = -\frac{6r^2}{\pi} \sum_{j=0}^{k} \alpha_j \frac{x_{n+k-j}^2}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4}, \quad i = \delta_{t0}(1)k.$$

This system of equations may be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{t0}(1)k$.

The following theorem characterizes the β-optimal multistep method (7) in $L^2(\hat{C}_r)$ space.

Theorem 3: The optimal multistep method (7) in which α_j's are prefixed, and optimization is done with respect to β_j's in $L^2(\hat{C}_r)$ space is characterized by that it is locally interpolatory for functions

$$\left\{ y_i(x) = \frac{x^2}{(r^2 - x\bar{x}_{n+k-i})^4}, \; i = \delta_{t0}(1)k \right\}.$$

Proof: The proof follows from Theorem 1 of Chapter 1, using the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

Corollary 1: If $x_{n+k-i} = 0$, for some $i = \delta_{t0}(1)k$, then the optimal method (7) is consistent.

Proof: The proof is similar to that of Corollary 1 of Chapter 4.

In the following tables we are presenting some numerical results for the β-optimal methods corresponding to Stormer's 1-point, Cowell's 3-points and Stormer's 5-points methods.

Table - 1a

x_n	$h^2\hat{\beta}_{1n}$	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.1091E-01	.6359E-03	.3283E-03
-1.6	.1050E-01	.3682E-04	.1918E-04
-1.5	.1031E-01	.4136E-05	.2222E-05
-1.4	.1021E-01	.7017E-06	.3929E-06
-1.3	.1015E-01	.1581E-06	.9278E-07
-1.2	.1011E-01	.4387E-07	.2709E-07
-1.1	.1008E-01	.1429E-07	.9312E-08
-1.0	.1006E-01	.5286E-08	.3647E-08
-.9	.1005E-01	.2173E-08	.1590E-08
-.8	.1004E-01	.9773E-09	.7587E-09
-.7	.1003E-01	.4755E-09	.3914E-09
-.6	.1002E-01	.2486E-09	.2164E-09
-.5	.1001E-01	.1393E-09	.1275E-09
-.4	.1001E-01	.8392E-10	.8000E-10
-.3	.1001E-01	.5477E-10	.5371E-10
-.2	.1000E-01	.3937E-10	.3918E-10
-.1	.1000E-01	.3183E-10	.3182E-10
.0	.1000E-01	.2957E-10	.2957E-10
.1	.1000E-01	.3183E-10	.3182E-10
.2	.1000E-01	.3937E-10	.3918E-10
.3	.1001E-01	.5477E-10	.5371E-10
.4	.1001E-01	.8392E-10	.8000E-10
.5	.1001E-01	.1393E-09	.1275E-09
.6	.1002E-01	.2486E-09	.2164E-09
.7	.1003E-01	.4755E-09	.3914E-09
.8	.1004E-01	.9773E-09	.7587E-09
.9	.1005E-01	.2173E-08	.1590E-08
1.0	.1006E-01	.5286E-08	.3647E-08
1.1	.1008E-01	.1429E-07	.9312E-08
1.2	.1011E-01	.4387E-07	.2709E-07
1.3	.1015E-01	.1581E-06	.9278E-07
1.4	.1021E-01	.7017E-06	.3929E-06
1.5	.1031E-01	.4136E-05	.2222E-05
1.6	.1050E-01	.3682E-04	.1918E-04
1.7	.1091E-01	.6359E-03	.3283E-03

Table for optimal β's and the square norm of LTE functionals for Størmer's 1-point method and the corresponding β-optimal method in $L^2(\mathrm{Cr})$-space, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; $\alpha_1=-1$, $\alpha_2=2$, $\alpha_3=-1$; $\beta_1=1$.

Table 1a shows that the optimal $\hat{\beta}_{1n}$'s are depending on nodal points and that in a neighborhood of the origin, the optimal $\hat{\beta}_{1n}$'s are nearly equal to usual β_1. At a point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$, at x=0, $\hat{\beta}_{1n}$ and β_1, as well as $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are numerically equal.

Table - 1b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	3	.275334E-02	2	.113882E-03
2	3	.137251E-02	3	.759100E-03
3	3	.425201E-02	3	.660814E-03
4	3	.226162E-02	3	.390301E-03
5	3	.547598E-02	3	.288221E-02
6	3	.110208E-02	3	.266344E-03
7	3	.269263E-03	3	.691810E-04
8	3	.152372E-02	2	.564563E-04
9	3	.829285E-03	2	.514084E-04
10	1	.122695E+00	1	.756851E-01
11	1	.163739E+00	1	.428818E-01
12	1	.159277E+00	1	.396641E-01
13	2	.262515E-03	2	.510016E-04
14	2	.190524E-03	2	.154842E-04
15	2	.279694E-03	2	.104465E-03
16	2	.207536E-03	2	.588077E-04
17	2	.237192E-05	2	.102788E-05
18	2	.200635E-04	2	.677542E-05
19	3	.486991E-02	3	.717588E-03
20	4	.601963E-02	3	.169067E-02
21	3	.473819E-02	3	.413338E-03
22	3	.268350E-02	3	.553183E-03
23	3	.474838E-02	3	.326285E-02
24	3	.924705E-03	3	.159715E-03

Table for number of iterations for convergence of the solution and the average discretisation errors using Størmer's 1-point usual and the corresponding β-optimal methods in $L^2(C_r)$-space, for 24 BVP-s.

The results of Table 1b are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1 for BVP's with equations 1-9, 19-24; and with r=2.8, a=-2.1, b=2.1, n=42, h=.1 for BVP's with equations 10-18. The numerical results show that this β-optimal method is two decimal places better on equation 8; one decimal place better on equations 1-4,6,7,9-14, 16,18,19,21 and 22, and just better on equations 5,15,17,20,23 and 24.

Table - 2a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.6057E-03	.9298E-02	-.1741E-03	.9730E-02	.2487E-04	.1748E-05
-1.6	.6882E-03	.8839E-02	.3942E-03	.9922E-02	.4108E-06	.3551E-07
-1.5	.7345E-03	.8640E-02	.5956E-03	.9970E-02	.1811E-07	.1882E-08
-1.4	.7630E-03	.8535E-02	.6884E-03	.9986E-02	.1452E-08	.1808E-09
-1.3	.7817E-03	.8473E-02	.7384E-03	.9993E-02	.1746E-09	.2615E-10
-1.2	.7948E-03	.8433E-02	.7683E-03	.9996E-02	.2820E-10	.5110E-11
-1.1	.8042E-03	.8406E-02	.7876E-03	.9998E-02	.5706E-11	.1260E-11
-1.0	.8113E-03	.8387E-02	.8007E-03	.9999E-02	.1380E-11	.3736E-12
-.9	.8168E-03	.8373E-02	.8100E-03	.9999E-02	.3865E-12	.1287E-12
-.8	.8210E-03	.8362E-02	.8168E-03	.1000E-01	.1223E-12	.5013E-13
-.7	.8244E-03	.8354E-02	.8218E-03	.1000E-01	.4305E-13	.2158E-13
-.6	.8270E-03	.8347E-02	.8256E-03	.1000E-01	.1664E-13	.1007E-13
-.5	.8291E-03	.8343E-02	.8283E-03	.1000E-01	.6986E-14	.5002E-14
-.4	.8307E-03	.8339E-02	.8303E-03	.1000E-01	.3262E-14	.2701E-14
-.3	.8319E-03	.8336E-02	.8317E-03	.1000E-01	.1700E-14	.1565E-14
-.2	.8327E-03	.8335E-02	.8326E-03	.1000E-01	.1011E-14	.9879E-15
-.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.6583E-15	.6567E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.5686E-15	.5686E-15
.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.5920E-15	.5904E-15
.2	.8326E-03	.8335E-02	.8327E-03	.1000E-01	.9090E-15	.8863E-15
.3	.8317E-03	.8336E-02	.8319E-03	.1000E-01	.1656E-14	.1520E-14
.4	.8303E-03	.8339E-02	.8307E-03	.1000E-01	.3280E-14	.2718E-14
.5	.8283E-03	.8343E-02	.8291E-03	.1000E-01	.7039E-14	.5055E-14
.6	.8256E-03	.8347E-02	.8270E-03	.1000E-01	.1669E-13	.1013E-13
.7	.8218E-03	.8354E-02	.8244E-03	.1000E-01	.4311E-13	.2164E-13
.8	.8168E-03	.8362E-02	.8210E-03	.1000E-01	.1223E-12	.5009E-13
.9	.8100E-03	.8373E-02	.8168E-03	.9999E-02	.3864E-12	.1286E-12
1.0	.8007E-03	.8387E-02	.8113E-03	.9999E-02	.1380E-11	.3736E-12
1.1	.7876E-03	.8406E-02	.8042E-03	.9998E-02	.5706E-11	.1260E-11
1.2	.7683E-03	.8433E-02	.7948E-03	.9996E-02	.2820E-10	.5110E-11
1.3	.7384E-03	.8473E-02	.7817E-03	.9993E-02	.1746E-09	.2615E-10
1.4	.6884E-03	.8535E-02	.7630E-03	.9986E-02	.1452E-08	.1808E-09
1.5	.5956E-03	.8640E-02	.7345E-03	.9970E-02	.1811E-07	.1882E-08
1.6	.3942E-03	.8839E-02	.6882E-03	.9922E-02	.4108E-06	.3551E-07
1.7	-.1741E-03	.9298E-02	.6057E-03	.9730E-02	.2487E-04	.1748E-05

Optimal β's, their row-sum and the square norm of LTE functionals for Cowell's 3-points usual and the corresponding β-optimal methods in $L^2(C_r)$-space, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; $\beta_0=.083333$, $\beta_1=.833333$, $\beta_2=.083333$.

Table 2a shows that the optimal $\hat{\beta}_{in}$'s are depending on the nodal points and that at a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$. In a neighborhood of the origin, the optimal $\hat{\beta}_{in}$'s are nearly equal to the corresponding usual β_i's, and $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are very close.

Table - 2b(i)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.283465E-04
2	2	.610703E-04	2	.535678E-04
3	3	.430195E-03	2	.221408E-05
4	2	.133292E-03	2	.395361E-04
5	2	.348263E-03	2	.228185E-03
6	3	.127772E-03	2	.692163E-05
7	2	.313175E-04	2	.211398E-05
8	2	.133523E-03	2	.121197E-04
9	2	.735570E-04	2	.265589E-05
10	1	.506252E-03	1	.209051E-02
11	1	.351768E-03	1	.134703E-01
12	1	.331492E-03	1	.132998E-01
13	2	.698086E-06	2	.363818E-04
14	2	.451879E-06	2	.328348E-04
15	2	.869978E-06	2	.262075E-04
16	2	.592198E-06	2	.235926E-04
17	1	.544969E-08	2	.101327E-06
18	1	.382493E-07	2	.105808E-05
19	3	.509406E-03	2	.234311E-04
20	3	.464907E-03	2	.197006E-04
21	2	.304134E-03	2	.737658E-04
22	2	.208304E-03	2	.553184E-04
23	2	.300455E-03	2	.226000E-03
24	2	.287372E-04	2	.394222E-04

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods in $L^2(C_r)$-space, for 24 BVP-s.

Numerical results of Table 2b(i) are obtained with r=2.01, a=-1.8, b=1.8, n=36 and h=.1 revealing that as compared to usual method, β-optimal method performs better on BVP's with equations 1-9 and 19-23, but worse on BVP's with equations 10-18 and 24 .

The results of the following Table 2b(ii) are obtained with r=2.8, a=-2.1, b=2.1, n=42, h=.1 for BVP's with equations 10-18, and with r=2.01, a=-1.9, b=1.9, n=38, h=.1 for BVP with equation 24. Tables 2b(i) and 2b(ii) reveal that as compared to usual method, β-optimal method for BVP is one decimal place better on eqns. 1,3,4,6-10,13-22 and just better on eqns. 2,5,11,12,23,24.

Table - 2b(ii)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
10	1	.170782E-02	1	.149522E-03
11	1	.738872E-03	1	.133189E-03
12	1	.718937E-03	1	.125355E-03
13	2	.298705E-05	1	.276705E-07
14	2	.167071E-05	1	.306032E-06
15	2	.392662E-05	2	.556663E-06
16	2	.236517E-05	1	.128682E-06
17	1	.257920E-07	1	.668273E-08
18	1	.151826E-06	1	.455183E-07
24	3	.210510E-03	3	.115611E-03

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods in $L^2(C_r)$-space, for BVP-s 10-18 and 24.

Table - 2c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.155059E-02
2	4	.250457E-02	4	.174033E-02
3	8	.760039E-01	4	.753252E-03
4	5	.132805E-01	4	.279643E-02
5	4	.716823E-02	4	.478021E-02
6	5	.356402E-02	4	.208882E-03
7	4	.354625E-03	3	.302951E-04
8	4	.211573E-02	3	.182664E-03
9	3	.604542E-03	2	.232164E-05
10	4	.119641E-01	4	.455832E-02
11	4	.130464E+00	4	.353892E-02
12	4	.129361E+00	4	.393477E-02
13	2	.128426E-05	1	.943582E-07
14	2	.831124E-06	1	.197656E-06
15	2	.193794E-05	1	.276215E-06
16	2	.130401E-05	1	.857718E-07
17	1	.456442E-08	1	.705316E-09
18	1	.343343E-07	1	.186947E-08
19	11	.103867E+00	5	.729780E-02
20	4	.188589E-02	3	.195450E-03
21	4	.112364E-02	3	.382116E-03
22	5	.115497E-01	4	.401051E-02
23	4	.610397E-02	4	.385898E-02
24	3	.542588E-04	3	.128426E-03

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods in $L^2(C_r)$-space, for 24 IVP-s.

The numerical results of Table 2c are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1 for IVP's with equations 1-9 and 19-24 and with r=2.7, a=-1.4, b=1.4, n=28, h=.1 for IVP's with equations 10-18. The optimal method is performing worse on equation 24 compared to the usual method. But in larger interval, say, a = -1.9, b = 1.9 and r = 2.01, n=38, h=.1, it gives favorable results where also the number of iterations for convergence of solution for usual method is becoming high. The results are given below.

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
24:	31	.7966732E-02	4	.327223E-02

Overall, as compared to the usual method, β-optimal method is two decimal places better for IVP's with equations 3,9,11-13,16,19; one decimal place better for IVP's with equations 1,4,6-8,10,15,17, 18,20-22; and just better for IVP's with equations 2,5,14,23 and 24.

In Tables 3a, 3b and 3c we are presenting the numerical results for the β-optimal method corresponding to Stormer's 5-points usual method. From Table 3a it is seen that the optimal $\hat{\beta}_{1n}$'s are depending on the nodal points and in a neighborhood of the origin, the optimal $\hat{\beta}_{1n}$'s are close to the corresponding usual β_1's. From table 3b, it is seen that at a general point x_n, $\|\hat{T}_n\|^2 \leq \|T_n\|^2$. At the beginning of Table 3b, $\|\hat{T}_n\|^2$ is much less than $\|T_n\|^2$compared to the end of this table, what is seen from the corresponding graphs also.

Table - 3a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	$h^2\hat{\beta}_{3n}$	$h^2\hat{\beta}_{4n}$
-1.3	.9957E-02	-.3300E-03	.3827E-03	-.5852E-04	.2790E-05
-1.2	.1027E-01	-.8884E-03	.7295E-03	-.1463E-03	.1027E-04
-1.1	.1054E-01	-.1436E-02	.1133E-02	-.2715E-03	.2395E-04
-1.0	.1077E-01	-.1959E-02	.1567E-02	-.4269E-03	.4400E-04
-.9	.1097E-01	-.2456E-02	.2021E-02	-.6068E-03	.7008E-04
-.8	.1115E-01	-.2930E-02	.2486E-02	-.8068E-03	.1018E-03
-.7	.1131E-01	-.3384E-02	.2959E-02	-.1024E-02	.1388E-03
-.6	.1146E-01	-.3818E-02	.3437E-02	-.1256E-02	.1806E-03
-.5	.1159E-01	-.4235E-02	.3917E-02	-.1500E-02	.2270E-03
-.4	.1172E-01	-.4637E-02	.4399E-02	-.1756E-02	.2778E-03
-.3	.1183E-01	-.5027E-02	.4883E-02	-.2023E-02	.3329E-03
-.2	.1194E-01	-.5408E-02	.5374E-02	-.2303E-02	.3927E-03
-.1	.1205E-01	-.5785E-02	.5873E-02	-.2597E-02	.4577E-03
.0	.1215E-01	-.6161E-02	.6388E-02	-.2910E-02	.5286E-03
.1	.1226E-01	-.6543E-02	.6923E-02	-.3244E-02	.6068E-03
.2	.1236E-01	-.6934E-02	.7488E-02	-.3606E-02	.6938E-03
.3	.1246E-01	-.7342E-02	.8092E-02	-.4003E-02	.7917E-03
.4	.1257E-01	-.7772E-02	.8746E-02	-.4445E-02	.9036E-03
.5	.1268E-01	-.8235E-02	.9468E-02	-.4945E-02	.1034E-02
.6	.1280E-01	-.8739E-02	.1028E-01	-.5521E-02	.1187E-02
.7	.1292E-01	-.9300E-02	.1120E-01	-.6198E-02	.1373E-02
.8	.1306E-01	-.9936E-02	.1228E-01	-.7011E-02	.1603E-02
.9	.1322E-01	-.1067E-01	.1357E-01	-.8014E-02	.1895E-02
1.0	.1340E-01	-.1154E-01	.1515E-01	-.9284E-02	.2277E-02
1.1	.1361E-01	-.1260E-01	.1714E-01	-.1095E-01	.2796E-02
1.2	.1386E-01	-.1393E-01	.1975E-01	-.1321E-01	.3530E-02
1.3	.1417E-01	-.1564E-01	.2328E-01	-.1643E-01	.4622E-02
1.4	.1457E-01	-.1795E-01	.2833E-01	-.2127E-01	.6348E-02
1.5	.1509E-01	-.2127E-01	.3605E-01	-.2915E-01	.9325E-02
1.6	.1583E-01	-.2642E-01	.4908E-01	-.4348E-01	.1512E-01
1.7	.1699E-01	-.3546E-01	.7451E-01	-.7422E-01	.2866E-01
1.8	.1909E-01	-.5482E-01	.1375E+00	-.1605E+00	.7109E-01

Table for optimal β's of the β-optimal method in $L^2(\hat{C}r)$-space corresponding to Stormer's 5-points usual method, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=1.2458$, $\beta_1=-.73333$, $\beta_2=.80833$, $\beta_3=-.4$, $\beta_4=.079167$.

Table - 3b

x	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.300	.258049E-03	.848220E-09
-1.200	.645653E-05	.123405E-09
-1.100	.356124E-06	.242352E-10
-1.000	.322349E-07	.615723E-11
-.900	.412492E-08	.194613E-11
-.800	.683616E-09	.740131E-12
-.700	.138693E-09	.329199E-12
-.600	.331516E-10	.167333E-12
-.500	.908783E-11	.954836E-13
-.400	.280310E-11	.603542E-13
-.300	.960427E-12	.419738E-13
-.200	.363022E-12	.318556E-13
-.100	.151519E-12	.262557E-13
.000	.708613E-13	.233946E-13
.100	.388029E-13	.225770E-13
.200	.270623E-13	.235053E-13
.300	.266105E-13	.265867E-13
.400	.370089E-13	.326048E-13
.500	.662970E-13	.434402E-13
.600	.139816E-12	.631345E-13
.700	.331589E-12	.100957E-12
.800	.868695E-12	.178863E-12
.900	.250916E-11	.354900E-12
1.000	.804176E-11	.800682E-12
1.100	.289479E-10	.209293E-11
1.200	.119190E-09	.650386E-11
1.300	.575983E-09	.249012E-10
1.400	.338795E-08	.123458E-09
1.500	.255763E-07	.851351E-09
1.600	.268741E-06	.909690E-08
1.700	.449456E-05	.179916E-06
1.800	.153874E-03	.919094E-05

Table for square norm of local truncation error functionals in $L^2(C_r)$ space, for Stormer's 5-points usual and the corresponding β-optimal methods, at the nodal points with r=2.01, a=-1.8, b=1.8, n=36, h=.1.

The results of Table 3c are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1 for IVP's with equations 1-9 and 19-24; and with r=2.8, a=-2.1, b=2.1, n=42, h=.1 for IVP's with equations 10-18. As compared to usual method the optimal method is four decimal places better on equations 10, 11; three decimal places better on equations 3,6,8,9, 15,19; two decimal places better on equations

1,4,5,7,12-14,16-18,20-22 and one decimal place better on equations 2,23 and 24.

Table - 3c

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.304356E-01	.171511E-03
2	.632144E-02	.142098E-03
3	.167084E+00	.169000E-03
4	.289167E-01	.177737E-03
5	.186264E-01	.539045E-03
6	.748945E-02	.721988E-05
7	.854658E-03	.239009E-05
8	.515672E-02	.441774E-05
9	.163408E-02	.716423E-05
10	.402219E+02	.307110E-02
11	.670431E+02	.954700E+00
12	.670732E+02	.792798E+00
13	.635226E-03	.660198E-05
14	.266670E-03	.770471E-05
15	.152962E-02	.122524E-05
16	.700262E-03	.423805E-05
17	.148635E-05	.114005E-07
18	.672210E-05	.512201E-07
19	.246038E+00	.569904E-03
20	.415804E-02	.253098E-04
21	.282785E-02	.291817E-04
22	.253443E-01	.177735E-03
23	.161435E-01	.170197E-02
24	.151126E-03	.111921E-04

Table for number of iterations for convergence of solution and the average discretisation errors using Stormer's 5-points usual and the corresponding β-optimal methods in $L^2(\hat{C}_r)$-space, for 24 IVP-s.

In $L^2(\hat{C}_r)$ space, to determine the optimal coefficients $\hat{\alpha}_{i,n}$, i = 0(1)k, of an α -optimal multistep method

$$\sum_{j=0}^{k} \hat{\alpha}_{j,n} y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0, \tag{9}$$

where β_j's are prefixed according to some consistent and stable known usual method with highest degree polynomial precision. With reference to equation (13) of Chapter 1, we have the system of

normal equations given by

$$\hat{C}\,\hat{a} = \hat{d},$$

where

$$\hat{a} = \left(\hat{\alpha}_{0,n}, \ldots\ldots\ldots, \hat{\alpha}_{k,n} \right)^T,$$

$$\hat{c}_{ij} = \frac{r^2}{\pi} \frac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}, \quad i, j = 0(1)k,$$

and $$\hat{d}_i = -\frac{6r^2}{\pi} h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \frac{\bar{x}^2_{n+k-i}}{(r^2 - \bar{x}_{n+k-i}x_{n+k-j})^4}, \quad i = 0(1)k.$$

This system of equations can be solved for $\hat{\alpha}_{j,n}$, $j = 0(1)k$.

The following theorem characterizes the α-optimal multistep method (9) in $L^2(\hat{C}_r)$ space.

<u>Theorem 4:</u> The optimal multistep method (9) in which β_j's are prefixed and optimization is done with respect to α_j's in $L^2(\hat{C}_r)$ space, is characterized by that it is locally interpolatory for functions

$$\left\{ y_i(x) = \frac{1}{(r^2 - x\bar{x}_{n+k-i})^2}, \ i = 0(1)k \right\}.$$

<u>Proof:</u> The proof follows from Theorem 2 of Chapter 1 and using the definitions of $K(z,\bar{t})$ and $D2(t,\bar{z})$ from (4) and (5).

<u>Remark:</u> If $x_{n+k-i} = 0$, for some $i = 0(1)k$, then the α-optimal method (9) is locally interpolatory for constants, which in other words tells that $\sum_{j=0}^{k} \hat{\alpha}_{j,n} = 0$.

Table - 4a

x_n	$\hat{\alpha}_{0n}$	$\hat{\alpha}_{1n}$	$\hat{\alpha}_{2n}$	r-sum	$\Vert T_n\Vert^2$	$\Vert\hat{T}_n\Vert^2$
-1.5	-.1001E+01	.2003E+01	-.1002E+01	-.2471E-04	.1814E-08	.1500E-08
-1.4	-.1001E+01	.2001E+01	-.1001E+01	-.7565E-05	.2102E-09	.1806E-09
-1.3	-.1000E+01	.2001E+01	-.1000E+01	-.2567E-05	.3298E-10	.2934E-10
-1.2	-.1000E+01	.2000E+01	-.1000E+01	-.9309E-06	.6519E-11	.5973E-11
-1.1	-.1000E+01	.2000E+01	-.1000E+01	-.3514E-06	.1546E-11	.1452E-11
-1.0	-.1000E+01	.2000E+01	-.1000E+01	-.1349E-06	.4249E-12	.4072E-12
-.9	-.1000E+01	.2000E+01	-.1000E+01	-.5161E-07	.1322E-12	.1286E-12
-.8	-.1000E+01	.2000E+01	-.1000E+01	-.1924E-07	.4571E-13	.4498E-13
-.7	-.1000E+01	.2000E+01	-.1000E+01	-.6806E-08	.1738E-13	.1724E-13
-.6	-.1000E+01	.2000E+01	-.1000E+01	-.2208E-08	.7163E-14	.7133E-14
-.5	-.1000E+01	.2000E+01	-.1000E+01	-.6250E-09	.3187E-14	.3198E-14
-.4	-.1000E+01	.2000E+01	-.1000E+01	-.1422E-09	.1527E-14	.1520E-14
-.3	-.1000E+01	.2000E+01	-.1000E+01	-.2226E-10	.8361E-15	.8161E-15
-.2	-.1000E+01	.2000E+01	-.1000E+01	-.1637E-11	.5326E-15	.5298E-15
-.1	-.1000E+01	.2000E+01	-.1000E+01	-.4441E-15	.3779E-15	.3609E-15
.0	-.1000E+01	.2000E+01	-.1000E+01	.0000E+00	.3171E-15	.3250E-15
.1	-.1000E+01	.2000E+01	-.1000E+01	-.2220E-15	.3249E-15	.3231E-15
.2	-.1000E+01	.2000E+01	-.1000E+01	-.1642E-11	.4266E-15	.4329E-15
.3	-.1000E+01	.2000E+01	-.1000E+01	-.2226E-10	.7830E-15	.7775E-15
.4	-.1000E+01	.2000E+01	-.1000E+01	-.1422E-09	.1563E-14	.1553E-14
.5	-.1000E+01	.2000E+01	-.1000E+01	-.6250E-09	.3214E-14	.3196E-14
.6	-.1000E+01	.2000E+01	-.1000E+01	-.2208E-08	.7207E-14	.7181E-14
.7	-.1000E+01	.2000E+01	-.1000E+01	-.6806E-08	.1733E-13	.1721E-13
.8	-.1000E+01	.2000E+01	-.1000E+01	-.1924E-07	.4568E-13	.4495E-13
.9	-.1000E+01	.2000E+01	-.1000E+01	-.5161E-07	.1322E-12	.1287E-12
1.0	-.1000E+01	.2000E+01	-.1000E+01	-.1349E-06	.4249E-12	.4072E-12
1.1	-.1000E+01	.2000E+01	-.1000E+01	-.3514E-06	.1546E-11	.1452E-11
1.2	-.1000E+01	.2000E+01	-.1000E+01	-.9309E-06	.6519E-11	.5973E-11
1.3	-.1000E+01	.2001E+01	-.1000E+01	-.2567E-05	.3298E-10	.2934E-10
1.4	-.1001E+01	.2001E+01	-.1001E+01	-.7565E-05	.2102E-09	.1806E-09
1.5	-.1002E+01	.2003E+01	-.1001E+01	-.2471E-04	.1814E-08	.1500E-08

Table for optimal α's, their row-sum and the square norm of local truncation error functionals for Cowell's 3-points usual and the corresponding β-optimal methods, in $L^2(C_r)$-space, at the nodal points, with r=2.1, a=-1.8, b=1.8, n=36, h=.1; $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; and $\beta_0=.083333$, $\beta_1=.833333$, $\beta_2=.083333$.

Table 4a shows that the optimal $\hat{\alpha}_{in}$'s are varying from point to point and they are very close to usual α_i's, at x=0 $\hat{\alpha}_{in}$'s are almost equal to α_i's; i=1,2,3. At a general point x_n, $\Vert\hat{T}_n\Vert^2\le\Vert T_n\Vert^2$, except at x=0, where the errors are of the order of 10^{-15}. Although the numerical calculations are done in double precision, such small

numbers are not so reliable. The reversal of the inequality at x = 0, in small numbers must be because of round-offs.

Table - 4b(i)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.241691E-04	2	.106158E-04
2	2	.102218E-04	2	.186843E-05
3	2	.417599E-04	2	.304933E-04
4	2	.198576E-04	2	.114593E-04
5	2	.392783E-04	2	.744216E-04
6	2	.108795E-04	2	.726836E-05
7	2	.246490E-05	2	.141227E-05
8	2	.128880E-04	2	.247714E-05
9	2	.658772E-05	1	.150434E-06
10	1	.111844E-02	1	.877442E-03
11	1	.575402E-03	1	.205577E-03
12	1	.555353E-03	1	.190362E-03
13	2	.174323E-05	2	.490685E-06
14	2	.103607E-05	1	.129003E-06
15	2	.224814E-05	2	.154660E-05
16	2	.142465E-05	2	.837506E-06
17	1	.146848E-07	1	.114576E-08
18	1	.920340E-07	1	.158628E-06
19	2	.459516E-04	2	.130596E-04
20	2	.396036E-04	2	.612652E-05
21	2	.299086E-04	2	.190148E-04
22	2	.218887E-04	2	.186571E-04
23	2	.363654E-04	2	.105602E-03
24	2	.106490E-05	2	.170235E-04

Table - 4b(ii)

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
5	1	.139188E-05	1	.130059E-05
18	1	.183027E-07	1	.455087E-08
23	2	.425829E-05	2	.423013E-05
24	1	.146241E-05	1	.146155E-05

Tables for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual and the corresponding α-optimal methods in $L^2(C_r)$-space, on 24 BVP-s.

The results of Table 4b(i) are obtained with r=2.1, a=-1.6, b=1.6, n=32, h=.1 for BVP's with equations 1-9 and 19-24 and with r=2.8, a=-2, b=2, n=40, h=.1 for equations 10-18. But still the

α-optimal method is producing worse results for BVP's with equations 5,18,23 and 24. Apparently it seems that, this situation happens because the singularities of the solutions of the differential equations 5,18,23 and 24 are not so pronounced. However with the same r, r=2.01, but in smaller interval, viz., a=-1, b=1 with n=20, α-optimal method gives just better result for equation 5, and with the same r, r=2.01, but in more reduced interval viz., a=-.6, b=.6 with n=12, the α-optimal method gives just better results for equations 23 and 24. With r=2.8, in an interval a=-1.6, b=1.6 with n=32, h=.1 α-optimal method is producing better result on equation 18 and these results are shown in Table 4b(ii).

In $L^2(\hat{C}_r)$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, i = $\delta_{to}(1)k$ of β-optimal multistep method (7) subject to the condition

(10) $$\sum_{j=\delta_{to}}^{k} \hat{\beta}_{j,n} = 1,$$

where α_j's are prefixed according to some consistent and stable known usual method (8) with highest degree polynomial precision, with reference to equation (15) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where

$$\hat{b} = h^2\left(\hat{\beta}_{\delta_{to},n},\,.......,\hat{\beta}_{k-1,n}\right)^T,$$

$$\hat{c}_{ij} = \frac{12r^2}{\pi} \frac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4}\left[1 + \frac{8x_{n+k-j}\bar{x}_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})} + \frac{10x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}\right]$$

$$- \frac{12r^2}{\pi} \frac{1}{(r^2 - x_{n+k-j}\bar{x}_n)^4}\left[1 + \frac{8x_{n+k-j}\bar{x}_n}{(r^2 - x_{n+k-j}\bar{x}_n)} + \frac{10x^2_{n+k-j}\bar{x}^2_n}{(r^2 - x_{n+k-j}\bar{x}_n)^2}\right]$$

$$- \frac{12r^2}{\pi} \frac{1}{(r^2 - x_n\bar{x}_{n+k-i})^4}\left[1 + \frac{8x_n\bar{x}_{n+k-i}}{(r^2 - x_n\bar{x}_{n+k-i})} + \frac{10x^2_n\bar{x}^2_{n+k-i}}{(r^2 - x_n\bar{x}_{n+k-i})^2}\right]$$

$$+ \frac{12r^2}{\pi} \frac{1}{(r^2 - x_n\bar{x}_n)^4}\left[1 + \frac{8x_n\bar{x}_n}{(r^2 - x_n\bar{x}_n)} + \frac{10x^2_n\bar{x}^2_n}{(r^2 - x_n\bar{x}_n)^2}\right], \quad i,j = \delta_{to}(1)k-1,$$

and

$$\hat{d}_i = -\frac{6r^2}{\pi} \sum_{j=0}^{k} \alpha_j \left\{\frac{x^2_{n+k-j}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4} - \frac{x^2_{n+k-j}}{(r^2 - x_{n+k-j}\bar{x}_n)^4}\right\}$$

$$- \frac{12r^2}{\pi} h^2 \left[\frac{1}{(r^2 - x_n\bar{x}_{n+k-i})^4}\left\{1 + \frac{8x_n\bar{x}_{n+k-i}}{(r^2 - x_n\bar{x}_{n+k-i})} + \frac{10x^2_n\bar{x}^2_{n+k-i}}{(r^2 - x_n\bar{x}_{n+k-i})^2}\right\}\right.$$

$$\left. - \frac{1}{(r^2 - x_n\bar{x}_n)^4}\left\{1 + \frac{8x_n\bar{x}_n}{(r^2 - x_n\bar{x}_n)} + \frac{10x^2_n\bar{x}^2_n}{(r^2 - x_n\bar{x}_n)^2}\right\}\right], \qquad i = \delta_{to}(1)k-1.$$

This system of equations may be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{to}(1)k-1$.

The following theorem characterizes the β-optimal multistep method (7) in $L^2(\hat{C}_r)$ space subject to the condition (10).

Theorem 5: The optimal multistep method (7) in which α_j's are prefixed and β_j's are optimized in $L^2(\hat{C}_r)$ space, subject to the condition (10) is characterized by that it is locally interpolatory for functions

$$\left\{y_i(x) = \frac{x^2}{(r^2 - x\bar{x}_{n+k-i})^4} - \frac{x^2}{(r^2 - x\bar{x}_n)^4},\ i = \delta_{to}(1)k-1\right\}.$$

Proof: The proof follows from Theorem 3 of Chapter 1, and the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

In $L^2(\hat{C}_r)$ space, we have to determine the optimal coefficients $\hat{\alpha}_{i,n}$, $i = 0(1)k$, and $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k-1$ of an (α,β)-optimal multistep method

$$\sum_{j=0}^{k} \hat{\alpha}_{j,n} y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} f_{n+k-j} = 0, \tag{11}$$

subject to the condition (10). With reference to equation (18) and (19) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where

$$\hat{b} = \left(\hat{\alpha}_{0,n},\ldots\ldots,\hat{\alpha}_{k,n},h^2\hat{\beta}_{\delta_{t0},n},\ldots\ldots,h^2\hat{\beta}_{k-1,n}\right)^T,$$

$$\hat{C}_{ij} = \frac{r^2}{\pi(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}, \quad i\ ,\ j = 0(1)k,$$

$$\hat{C}_{ij} = \frac{6r^2}{\pi}\left[\frac{\bar{x}^2_{n+k-i}}{(r^2-\bar{x}_{n+k-i}x_{n+k-j})^4} - \frac{\bar{x}^2_{n+k-i}}{(r^2-\bar{x}_{n+k-i}x_n)^4}\right], \quad i=0(1)k,\ j=k+1(1)2k+1-\delta_{t0},$$

$$\hat{C}_{ij} = \frac{6r^2}{\pi}\left[\frac{x^2_{n+k-j}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^4} - \frac{x^2_{n+k-j}}{(r^2-x_{n+k-j}\bar{x}_n)^4}\right]; \quad i=k+1(1)2k+1-\delta_{t0},\ j=0(1)k$$

$$\hat{C}_{ij} = \frac{12r^2}{\pi}\frac{1}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^4}\left[1+\frac{8x_{n+k-j}\bar{x}_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})}+\frac{10x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2-x_{n+k-j}\bar{x}_{n+k-i})^2}\right]$$

$$-\frac{12r^2}{\pi}\frac{1}{(r^2-x_{n+k-j}\bar{x}_n)^4}\left[1+\frac{8x_{n+k-j}\bar{x}_n}{(r^2-x_{n+k-j}\bar{x}_n)}+\frac{10x^2_{n+k-j}\bar{x}^2_n}{(r^2-x_{n+k-j}\bar{x}_n)^2}\right]$$

$$- \frac{12r^2}{\pi}\, \frac{1}{(r^2-x_n\bar{x}_{n+k-i})^4}\left[1+\frac{8x_n\bar{x}_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})}+\frac{10x_n^2\bar{x}_{n+k-i}^2}{(r^2-x_n\bar{x}_{n+k-i})^2}\right]$$

$$+ \frac{12r^2}{\pi}\, \frac{1}{(r^2-x_n\bar{x}_n)^4}\left[1+\frac{8x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{10x_n^2\bar{x}_n^2}{(r^2-x_n\bar{x}_n)^2}\right],\quad i,j = k+1(1)2k+1-\delta_{to},$$

and

$$\hat{d}_i = h^2\, \frac{6r^2}{\pi}\, \frac{\bar{x}_{n+k-i}^2}{(r^2-\bar{x}_{n+k-i}x_n)^4},\qquad i = 0(1)k,$$

$$\hat{d}_i \;=\; -\; h^2\frac{12r^2}{\pi}\left[\frac{1}{(r^2-x_n\bar{x}_{n+k-i})^4}\left\{1+\frac{8x_n\bar{x}_{n+k-i}}{(r^2-x_n\bar{x}_{n+k-i})}+\frac{10x_n^2\bar{x}_{n+k-i}^2}{(r^2-x_n\bar{x}_{n+k-i})^2}\right\}\right.$$

$$\left.- \frac{1}{(r^2-x_n\bar{x}_n)^4}\left\{1+\frac{8x_n\bar{x}_n}{(r^2-x_n\bar{x}_n)}+\frac{10x_n^2\bar{x}_n^2}{(r^2-x_n\bar{x}_n)^2}\right\}\right],\quad i,j = k+1(1)2k+1-\delta_{to}.$$

The following theorem characterizes the (α,β)-optimal method (11) in $L^2(\hat{C}_r)$ space subject to the condition (10).

<u>Theorem 6</u>: The optimal multistep method (11) in which α_j's as well as β_j's are optimized in $L^2(\hat{C}_r)$ space, subject to the condition (10) is characterized by that it is locally interpolatory for functions $\{y_{1i}(x),\ i=\delta_{to}(1)k-1\} \cup \{y_{2i}(x),\ i=0(1)k-1\}$, where

$$y_{1i}(x) = \frac{x^2}{(r^2-x\bar{x}_{n+k-i})^4} - \frac{x^2}{(r^2-x\bar{x}_n)^4},\quad i = \delta_{to}(1)k-1$$

and $$y_{2i}(x) = \frac{1}{(r^2-x\bar{x}_{n+k-i})^2},\quad i = 0(1)k-1.$$

<u>Proof:</u> The proof follows from Theorem 4 of Chapter 1, and the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$ and $D2''(t,\bar{z})$ from (4), (5) and (6).

Table - 5a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.6432E-03	.8980E-02	.3767E-03	.1000E-01	.2487E-04	.2920E-05
-1.6	.7176E-03	.8672E-02	.6109E-03	.1000E-01	.4108E-06	.5854E-07
-1.5	.7565E-03	.8540E-02	.7039E-03	.1000E-01	.1811E-07	.2997E-08
-1.4	.7793E-03	.8471E-02	.7500E-03	.1000E-01	.1452E-08	.2751E-09
-1.3	.7938E-03	.8430E-02	.7761E-03	.1000E-01	.1746E-09	.3779E-10
-1.2	.8036E-03	.8404E-02	.7923E-03	.1000E-01	.2820E-10	.6988E-11
-1.1	.8106E-03	.8386E-02	.8031E-03	.1000E-01	.5706E-11	.1626E-11
-1.0	.8157E-03	.8374E-02	.8107E-03	.1000E-01	.1380E-11	.4550E-12
-.9	.8197E-03	.8364E-02	.8162E-03	.1000E-01	.3865E-12	.1484E-12
-.8	.8228E-03	.8357E-02	.8205E-03	.1000E-01	.1223E-12	.5502E-13
-.7	.8254E-03	.8351E-02	.8238E-03	.1000E-01	.4305E-13	.2277E-13
-.6	.8275E-03	.8346E-02	.8265E-03	.1000E-01	.1664E-13	.1034E-13
-.5	.8293E-03	.8342E-02	.8287E-03	.1000E-01	.6986E-14	.5053E-14
-.4	.8307E-03	.8339E-02	.8304E-03	.1000E-01	.3262E-14	.2708E-14
-.3	.8319E-03	.8336E-02	.8317E-03	.1000E-01	.1700E-14	.1565E-14
-.2	.8327E-03	.8335E-02	.8326E-03	.1000E-01	.1011E-14	.9879E-15
-.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.6583E-15	.6567E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.5686E-15	.5686E-15
.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.5920E-15	.5904E-15
.2	.8326E-03	.8335E-02	.8327E-03	.1000E-01	.9090E-15	.8863E-15
.3	.8317E-03	.8336E-02	.8319E-03	.1000E-01	.1656E-14	.1521E-14
.4	.8304E-03	.8339E-02	.8307E-03	.1000E-01	.3280E-14	.2725E-14
.5	.8287E-03	.8342E-02	.8293E-03	.1000E-01	.7039E-14	.5106E-14
.6	.8265E-03	.8346E-02	.8275E-03	.1000E-01	.1669E-13	.1039E-13
.7	.8238E-03	.8351E-02	.8254E-03	.1000E-01	.4311E-13	.2283E-13
.8	.8205E-03	.8357E-02	.8228E-03	.1000E-01	.1223E-12	.5497E-13
.9	.8162E-03	.8364E-02	.8197E-03	.1000E-01	.3864E-12	.1482E-12
1.0	.8107E-03	.8374E-02	.8157E-03	.1000E-01	.1380E-11	.4550E-12
1.1	.8031E-03	.8386E-02	.8106E-03	.1000E-01	.5706E-11	.1626E-11
1.2	.7923E-03	.8404E-02	.8036E-03	.1000E-01	.2820E-10	.6988E-11
1.3	.7761E-03	.8430E-02	.7938E-03	.1000E-01	.1746E-09	.3779E-10
1.4	.7500E-03	.8471E-02	.7793E-03	.1000E-01	.1452E-08	.2751E-09
1.5	.7039E-03	.8540E-02	.7565E-03	.1000E-01	.1811E-07	.2997E-08
1.6	.6109E-03	.8672E-02	.7176E-03	.1000E-01	.4108E-06	.5854E-07
1.7	.3767E-03	.8980E-02	.6432E-03	.1000E-01	.2487E-04	.2920E-05

Table for optimal β's, their row-sum and the square norm of local truncation error functionals for Cowell's 3-point usual method and the corresponding β-optimal method with restriction, in $L^2(\hat{C}_r)$-space, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; α_0=-1, α_1=2, α_2=-1; and β_0=.083333, β_1=.833333, β_2=.083333.

From Table 5a it is seen that the optimal $\hat{\beta}_{1n}$'s are depending on the nodal points and at a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$. In a neighborhood of the origin the optimal $\hat{\beta}_{1n}$'s are close to the

corresponding usual β_i's. At x=0, $\hat{\beta}_{in}$ and β_i, i=1,2,3, as well as $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are numerically equal.

Table - 5b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.813027E-04
2	2	.610703E-04	2	.499576E-04
3	3	.430195E-03	2	.109803E-03
4	2	.133292E-03	2	.603006E-04
5	2	.348263E-03	2	.199561E-03
6	3	.127772E-03	2	.321776E-04
7	2	.313175E-04	2	.797586E-05
8	2	.133523E-03	2	.446397E-04
9	2	.735570E-04	2	.246009E-04
10	1	.170782E-02	1	.190608E-03
11	1	.738872E-03	1	.298466E-03
12	1	.718937E-03	1	.288824E-03
13	2	.298705E-05	2	.116579E-05
14	2	.167071E-05	2	.728604E-06
15	2	.392662E-05	2	.137844E-05
16	2	.236517E-05	2	.827569E-06
17	1	.257920E-07	1	.948448E-08
18	1	.151826E-06	1	.700690E-07
19	3	.509406E-03	2	.133109E-03
20	3	.464907E-03	2	.125596E-03
21	2	.304134E-03	2	.116677E-03
22	2	.208304E-03	2	.799850E-04
23	2	.300455E-03	2	.163980E-03
24	2	.287372E-04	2	.161187E-04

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method with restriction in $L^2(\hat{C}_r)$-space, for 24 BVP-s.

Results in Table 5b are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1 for BVP's with equations 1-9 and 19-24 and with r=2.8, a=-2.1, b=2.1, n=42, h=.1 for BVP's with equations 10-18. Table 5b reveals that as compared to usual method β-optimal method with restriction for BVP is one decimal place better on equations 1,4,6-8,10,14,16-18,22; and just better on equations 2,3,5,9, 11-13,15,19-21,23 and 24.

Table - 5c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.485217E-02
2	4	.250457E-02	4	.173155E-02
3	8	.760039E-01	5	.173120E-01
4	5	.132805E-01	4	.509940E-02
5	4	.716823E-02	4	.423506E-02
6	5	.356402E-02	4	.963058E-03
7	4	.354625E-03	3	.100186E-03
8	4	.211573E-02	4	.750653E-03
9	3	.604542E-03	3	.220553E-03
10	4	.119641E-01	4	.513783E-02
11	4	.130464E+00	4	.753139E-02
12	4	.129361E+00	4	.746002E-02
13	2	.128426E-05	2	.551296E-06
14	2	.831124E-06	1	.360443E-06
15	2	.193794E-05	2	.805851E-06
16	2	.130401E-05	2	.530703E-06
17	1	.456442E-08	1	.398993E-09
18	1	.343343E-07	1	.277793E-08
19	11	.103867E+00	6	.200835E-01
20	4	.188589E-02	3	.484536E-03
21	4	.112364E-02	3	.397635E-03
22	5	.115497E-01	4	.409179E-02
23	4	.610397E-02	4	.357735E-02
24	3	.542588E-04	2	.685449E-05

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method with restriction in $L^2(\hat{C}_r)$-space, for 24 IVP-s.

The results of Table 5c are obtained with r=2.01, a=-1.7, b=1.7, n=34 and h=.1 for IVP's with equations 1-9 and 19-24 and with r=2.7, a=-1.4, b=1.4, n=28, h=.1 for IVP's with equations

10-18. Table 5c shows that as compared to usual method β-optimal method with restriction for IVP is two decimal places better on equations 11,12; one decimal place better on equations 1,4,6,8, 10, 12,15-22,24; and just better on equations 2,3,5,7,14 and 23.

5.4 Optimal multistep methods in $L^2(\hat{C}_r)$-space Interpolatory For Polynomials.

In section 4.4, we have discussed optimal multistep methods, in $H^2(C_r)$ space, interpolatory for polynomials of a certain degree. Similar to that methodology, β-optimal multistep method in $L^2(\hat{C}_r)$ space, interpolatory for polynomials of degree $q < k+\delta_{t1}+1$, is given by

$$(12)\qquad \sum_{j=0}^{k}\alpha_j y_{n+k-j} + h^2\sum_{j=0}^{q-2}\gamma_j^u \nabla^j f(x_{n+k-\delta_{t0}}, y_{n+k-\delta_{t0}}) = - h^2 \sum_{j=q-1}^{k-\delta_{t0}} \hat{\gamma}_{j,n}\nabla^j f(x_{n+k-\delta_{t0}}, y_{n+k-\delta_{t0}}),$$

with prefixed α_i's such that $\sum_{i=0}^{k}\alpha_i = 0$, $\sum_{i=0}^{k} i\alpha_i = 0$, and with prefixed γ_j^u, $j = 0(1)q-2$, as in the corresponding usual method. The optimal coefficients $\hat{\gamma}_{j,n}$, $j = q-1(1)k-\delta_{t0}$, are to satisfy the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d}^{\perp}$$

where

$$\hat{b} = \left(\hat{\gamma}_{q-1,n}, \hat{\gamma}_{q,n}, \ldots\ldots, \hat{\gamma}_{k-\delta_{t0},n}\right)^T,$$

$$\hat{c}_{ij} = h^2 \sum_{m=0}^{j}\sum_{l=0}^{i} (-1)^{l+m}\, {}^iC_l\, {}^jC_m \frac{12r^2}{\pi} \frac{1}{(r^2 - x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-l})^4}.$$

$$\cdot\left[1+\frac{8x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1}}{(r^2-x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1})}+\frac{10x^2_{n+k-\delta_{t0}-m}\bar{x}^2_{n+k-\delta_{t0}-1}}{(r^2-x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1})^2}\right],$$

and

$$\hat{d}_i = -\sum_{j=0}^{k}\alpha_j\sum_{l=0}^{i}(-1)^l\ {}^iC_l\frac{6r^2}{\pi}\frac{x^2_{n+k-j}}{(r^2-x_{n+k-j}\bar{x}_{n+k-\delta_{t0}-1})^4}$$

$$-h^2\sum_{j=0}^{q-2}\gamma^u_j\qquad\sum_{m=0}^{j}\sum_{l=0}^{i}(-1)^{l+m}\ {}^iC_l\ {}^jC_m\frac{12r^2}{\pi}\frac{1}{(r^2-x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1})^4}\cdot$$

$$\cdot\left[1+\frac{8x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1}}{(r^2-x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1})}+\frac{10x^2_{n+k-\delta_{t0}-m}\bar{x}^2_{n+k-\delta_{t0}-1}}{(r^2-x_{n+k-\delta_{t0}-m}\bar{x}_{n+k-\delta_{t0}-1})^2}\right]$$

$$i = q-1(1)k-\delta_{t0}.$$

Thus we get the following theorem.

Theorem 7: The optimal multistep method (12) interpolatory for polynomials of degree q is characterized by that it is locally interpolatory for functions

$$\{x^i;\ i = 1(1)q\}\cup\{h_i(x);\ i = q-1(1)k-\delta_{t0}\},$$

where $h_i(x) = \sum_{l=0}^{i}(-1)^l\ {}^iC_l\ \dfrac{x^2}{(r^2-x\bar{x}_{n+k-\delta_{t0}-1})^4}$.

In the following Tables 6a-6c we are presenting the numerical results for β-optimal method interpolatory for polynomials of degree 3 corresponding to Cowell's 3-points usual method. From Table 6a, it is clear that the optimal $\hat{\beta}_{in}$'s are depending on nodal points and at a general point x_n, $\|\hat{T}_n\|^2\le\|T_n\|^2$. In a neighborhood of the origin, the optimal $\hat{\beta}_{in}$'s are close to the corresponding usual β_i's; i=0,1,2; at x=0, they as well as $\|\hat{T}_n\|^2$ and $\|T_n\|^2$ are

numerically the same .

Table - 6a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.7126E-03	.8575E-02	.7126E-03	.1000E-01	.2487E-04	.6813E-05
-1.6	.7664E-03	.8467E-02	.7664E-03	.1000E-01	.4108E-06	.1306E-06
-1.5	.7911E-03	.8418E-02	.7911E-03	.1000E-01	.1811E-07	.6347E-08
-1.4	.8045E-03	.8391E-02	.8045E-03	.1000E-01	.1452E-08	.5509E-09
-1.3	.8126E-03	.8375E-02	.8126E-03	.1000E-01	.1746E-09	.7131E-10
-1.2	.8178E-03	.8364E-02	.8178E-03	.1000E-01	.2820E-10	.1238E-10
-1.1	.8214E-03	.8357E-02	.8214E-03	.1000E-01	.5706E-11	.2696E-11
-1.0	.8240E-03	.8352E-02	.8240E-03	.1000E-01	.1380E-11	.7036E-12
-.9	.8260E-03	.8348E-02	.8260E-03	.1000E-01	.3865E-12	.2133E-12
-.8	.8275E-03	.8345E-02	.8275E-03	.1000E-01	.1223E-12	.7338E-13
-.7	.8287E-03	.8343E-02	.8287E-03	.1000E-01	.4305E-13	.2818E-13
-.6	.8297E-03	.8341E-02	.8297E-03	.1000E-01	.1664E-13	.1193E-13
-.5	.8306E-03	.8339E-02	.8306E-03	.1000E-01	.6986E-14	.5487E-14
-.4	.8314E-03	.8337E-02	.8314E-03	.1000E-01	.3262E-14	.2809E-14
-.3	.8321E-03	.8336E-02	.8321E-03	.1000E-01	.1700E-14	.1582E-14
-.2	.8327E-03	.8335E-02	.8327E-03	.1000E-01	.1011E-14	.9892E-15
-.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.6583E-15	.6567E-15
.0	.8333E-03	.8333E-02	.8333E-03	.1000E-01	.5686E-15	.5686E-15
.1	.8331E-03	.8334E-02	.8331E-03	.1000E-01	.5920E-15	.5904E-15
.2	.8327E-03	.8335E-02	.8327E-03	.1000E-01	.9090E-15	.8876E-15
.3	.8321E-03	.8336E-02	.8321E-03	.1000E-01	.1656E-14	.1538E-14
.4	.8314E-03	.8337E-02	.8314E-03	.1000E-01	.3280E-14	.2826E-14
.5	.8306E-03	.8339E-02	.8306E-03	.1000E-01	.7039E-14	.5540E-14
.6	.8297E-03	.8341E-02	.8297E-03	.1000E-01	.1669E-13	.1198E-13
.7	.8287E-03	.8343E-02	.8287E-03	.1000E-01	.4311E-13	.2824E-13
.8	.8275E-03	.8345E-02	.8275E-03	.1000E-01	.1223E-12	.7334E-13
.9	.8260E-03	.8348E-02	.8260E-03	.1000E-01	.3864E-12	.2132E-12
1.0	.8240E-03	.8352E-02	.8240E-03	.1000E-01	.1380E-11	.7036E-12
1.1	.8214E-03	.8357E-02	.8214E-03	.1000E-01	.5706E-11	.2696E-11
1.2	.8178E-03	.8364E-02	.8178E-03	.1000E-01	.2820E-10	.1238E-10
1.3	.8126E-03	.8375E-02	.8126E-03	.1000E-01	.1746E-09	.7131E-10
1.4	.8045E-03	.8391E-02	.8045E-03	.1000E-01	.1452E-08	.5509E-09
1.5	.7911E-03	.8418E-02	.7911E-03	.1000E-01	.1811E-07	.6347E-08
1.6	.7664E-03	.8467E-02	.7664E-03	.1000E-01	.4108E-06	.1306E-06
1.7	.7126E-03	.8575E-02	.7126E-03	.1000E-01	.2487E-04	.6813E-05

Table for optimal β's, their row-sum and the square norm of local truncation error functionals, in $L^2(C_r)$ space, for Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; $\beta_0=.083333$, $\beta_1=.833333$, $\beta_2=.083333$; $\gamma_0=1$, $\gamma_1=-1$, $\gamma_2=1/12$.

Table - 6b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.240920E-04
2	2	.610703E-04	2	.461772E-04
3	3	.430195E-03	2	.121004E-04
4	2	.133292E-03	2	.642565E-04
5	2	.348263E-03	2	.120095E-03
6	3	.127772E-03	2	.101242E-04
7	2	.313175E-04	2	.245537E-05
8	2	.133523E-03	2	.124323E-04
9	2	.735570E-04	2	.670919E-05
10	1	.111844E-02	1	.279828E-03
11	1	.575402E-03	1	.505366E-03
12	1	.555353E-03	1	.503450E-03
13	2	.174323E-05	1	.234601E-06
14	2	.103607E-05	1	.312393E-07
15	2	.224814E-05	2	.561019E-06
16	2	.142465E-05	1	.199793E-06
17	1	.146848E-07	1	.143021E-08
18	1	.920340E-07	1	.154712E-07
19	3	.509406E-03	2	.175912E-04
20	3	.464907E-03	2	.150172E-04
21	2	.304134E-03	2	.432583E-04
22	2	.208304E-03	2	.307457E-04
23	2	.300455E-03	2	.132747E-03
24	2	.287372E-04	2	.102816E-05

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, in $L^2(C_r)$ space, for 24 BVP-s.

The numerical results of Table 6b are obtained for BVP's with equations 1-9 and 19-24 with r=2.01, a=-1.8, b=1.8, n=36, h=.1; and for BVP's with equations 10-18 with r=2.8, a=-2, b=2, n=40, h=.1. Table 6b reveals that as compared to usual method β-optimal method interpolatory for polynomials of degree 3 for BVP is two decimal places better on equation 14; one decimal place better on equations 1,3,4,6-10,13,15-17,19-22 and 24; and just better on equations 2,5,11,12,18 and 23.

Table - 6c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.105817E-02
2	4	.250457E-02	4	.154352E-02
3	8	.760039E-01	4	.902492E-03
4	5	.132805E-01	4	.450808E-02
5	4	.716823E-02	4	.233608E-02
6	5	.356402E-02	4	.353335E-03
7	4	.354625E-03	3	.357746E-04
8	4	.211573E-02	3	.150320E-03
9	3	.604542E-03	3	.405464E-04
10	4	.119641E-01	4	.625978E-02
11	4	.130464E+00	4	.830081E-02
12	4	.129361E+00	4	.893553E-02
13	2	.128426E-05	1	.145172E-06
14	2	.831124E-06	1	.182743E-07
15	2	.193794E-05	2	.456883E-06
16	2	.130401E-05	1	.213949E-06
17	1	.456442E-08	1	.264896E-09
18	1	.343343E-07	1	.107190E-07
19	11	.103867E+00	5	.436396E-02
20	4	.188589E-02	3	.112072E-03
21	4	.112364E-02	3	.129308E-03
22	5	.115497E-01	4	.139534E-02
23	4	.610397E-02	4	.245008E-02
24	3	.542588E-04	2	.422862E-05

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, in $L^2(C_r)$ space, for 24 IVP-s.

The results of Table 6c are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1 for IVP's with equations 1-9 and 19-24; and with r = 2.7, a=-1.4, b=1.4, n=28, h=.1 for IVP's with equations 10-18. Table 6c reveals that as compared to usual method, β-optimal method interpolatory for polynomials of degree 3 for IVP is two decimal places better on equation 3,11,12,19; one decimal place better on equations 1,4,6-10,13-17,20-22 and 24; and just better on equations 2,5,18 and 23.

Similar to the α-optimal multistep method in $H^2(C_r)$ space, interpolatory for polynomials of degree q, discussed in section 4.4, the α-optimal multistep method in $L^2(\hat{C}_r)$ space,

$$(13) \qquad \sum_{j=2}^{q} \gamma_j^u \nabla^j y_{n+k} + \sum_{j=q+1}^{k} \gamma_j \nabla^j y_{n+k} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0,$$

with prefixed β_j's and γ_j^u 's as in the corresponding usual method are to satisfy the system of normal equations

$$\hat{C}\,\hat{a} = \hat{d},$$

where

$$\hat{a} = \left(\hat{\gamma}_{q+1,n}, \ldots\ldots, \hat{\gamma}_{k,n}\right)^T,$$

$$\hat{C}_{ij} = \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\ {}^iC_l\ {}^jC_m \frac{r^2}{\pi} \frac{1}{(r^2 - x_{n+k-m}\bar{x}_{n+k-l})^2}, \quad i,j = q+1(1)k$$

$$\hat{d}_i = -\sum_{j=2}^{q} \gamma_j^u \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\ {}^iC_l\ {}^jC_m \frac{r^2}{\pi} \frac{1}{(r^2 - x_{n+k-m}\bar{x}_{n+k-l})^2}$$

$$- h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \sum_{l=0}^{i} (-1)^{l}\ {}^iC_l \frac{6r^2}{\pi} \frac{\bar{x}^2_{n+k-l}}{(r^2 - \bar{x}_{n+k-l}x_{n+k-j})^4}, \quad i = q+1(1)k.$$

Hence we get the following theorem.

<u>Theorem 8</u> : The optimal multistep method (13) interpolatory for polynomials of degree q is characterized by that it is locally interpolatory for functions

$$\{x^i;\ i = 1(1)q\} \cup \{\underline{h}_i(x);\ i = q+1(1)k\}$$

where $h_i(x) = \sum_{l=0}^{i} (-1)^l\ {}^iC_l \dfrac{1}{(r^2 - x\bar{x}_{n+k-l})^2}, \quad i = q+1(1)k.$

5.5 Optimal Multistep Methods in $L^2(\hat{C}_r)$-Space Interpolatory for a Set of Preassigned Functions.

To obtain the coefficients $\hat{\beta}^F_{j,n}$, $j = \delta_{t0}(1)k$ of a β-optimal multistep method

(14) $$\sum_{j=0}^{k} \alpha_j \, y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,n} \, f_{n+k-j} = 0,$$

in $L^2(\hat{C}_r)$ space with prefixed α_j's, interpolatory for q number of linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$, we have to solve a system of linear equations given in the matrix form as

$$\begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where $A = (A_{ij})$, $i,j = \delta_{t0}(1)k$, with

$$A_{ij} = \frac{12r^2}{\pi} \frac{1}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4} \cdot \left[1 + \frac{8x_{n+k-j}\bar{x}_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})} + \frac{10x^2_{n+k-j}\bar{x}^2_{n+k-i}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^2}\right], \quad i,\, j = \delta_{t0}(1)k,$$

$$F = (F_{ij})_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k}}, \qquad \text{with} \quad F_{ij} = f''_i\,(x_{n+k-j}),$$

$$b = h^2\left(\hat{\beta}^F_{\delta_{t0},n}, \hat{\beta}^F_{\delta_{t0}+1,n}, \ldots, \hat{\beta}^F_{k,n}\right)^T, \qquad \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q)^T,$$

$$c = \left(c_{\delta_{t0}}, c_{\delta_{t0}+1}, \ldots, c_k\right)^T, \text{ with } c_i = -\sum_{j=0}^{k} \alpha_j \frac{6r^2}{\pi} \frac{x^2_{n+k-j}}{(r^2 - x_{n+k-j}\bar{x}_{n+k-i})^4},$$

and

$$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T, \qquad \text{with } \tilde{f}_i = -\sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j}).$$

This method is characterized as follows.

Theorem 9: The β-optimal multistep method (14), in $L^2(\hat{C}_r)$ space, interpolatory for linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$ is characterized by that, it is locally interpolatory for the functions

$$\{f_1, f_2, \ldots, f_q\} \cup \{h_i,\ i = \delta_{t0}(1)k-q\},$$

where

$$h_i(x) = \frac{x^2}{(r^2 - x\bar{x}_{n+k-i})^4} - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1-\delta_{t0}} \frac{x^2}{(r^2 - x\bar{x}_{n+k-j})^4}$$

and

$$G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}},$$

where

$$P = \Big(f_i''\ (x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=k-q+1(1)k}} \quad \text{and} \quad E = \Big(f_i''\ (x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-q}}.$$

Proof: The proof follows from Theorem 8 of Chapter 1.

In the Tables 7a-7c we are presenting the numerical results for the β-optimal method interpolatory for linearly independent functions exp(1.6x) and exp(-1.6x). From Table 7a it is clear that the optimal $\hat{\beta}_{in}$'s are depending on the nodal points, and in a neighborhood of the origin the optimal $\hat{\beta}_{in}$'s are close to the corresponding usual β_i's. At at a general point x_n, $\|\hat{T}_n\|^2 \le \|T_n\|^2$, except at x=-.1, 0 and .1 which must be because of round-offs in the middle of the table.

Table - 7a

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.7	.7110E-03	.8581E-02	.7110E-03	.1000E-01	.2487E-04	.6670E-05
-1.6	.7646E-03	.8473E-02	.7646E-03	.1000E-01	.4108E-06	.1262E-06
-1.5	.7893E-03	.8423E-02	.7893E-03	.1000E-01	.1811E-07	.6040E-08
-1.4	.8027E-03	.8395E-02	.8027E-03	.1000E-01	.1452E-08	.5163E-09
-1.3	.8108E-03	.8379E-02	.8108E-03	.1000E-01	.1746E-09	.6589E-10
-1.2	.8161E-03	.8368E-02	.8161E-03	.1000E-01	.2820E-10	.1132E-10
-1.1	.8199E-03	.8361E-02	.8199E-03	.1000E-01	.5706E-11	.2449E-11
-1.0	.8226E-03	.8355E-02	.8226E-03	.1000E-01	.1380E-11	.6397E-12
-.9	.8248E-03	.8351E-02	.8248E-03	.1000E-01	.3865E-12	.1956E-12
-.8	.8266E-03	.8347E-02	.8266E-03	.1000E-01	.1223E-12	.6838E-13
-.7	.8281E-03	.8344E-02	.8281E-03	.1000E-01	.4305E-13	.2681E-13
-.6	.8294E-03	.8341E-02	.8294E-03	.1000E-01	.1664E-13	.1159E-13
-.5	.8305E-03	.8339E-02	.8305E-03	.1000E-01	.6986E-14	.5419E-14
-.4	.8314E-03	.8337E-02	.8314E-03	.1000E-01	.3262E-14	.2798E-14
-.3	.8321E-03	.8336E-02	.8321E-03	.1000E-01	.1700E-14	.1581E-14
-.2	.8326E-03	.8335E-02	.8326E-03	.1000E-01	.1011E-14	.9934E-15
-.1	.8329E-03	.8334E-02	.8329E-03	.1000E-01	.6583E-15	.6677E-15
.0	.8330E-03	.8334E-02	.8330E-03	.1000E-01	.5686E-15	.5828E-15
.1	.8329E-03	.8334E-02	.8329E-03	.1000E-01	.5920E-15	.6014E-15
.2	.8326E-03	.8335E-02	.8326E-03	.1000E-01	.9090E-15	.8918E-15
.3	.8321E-03	.8336E-02	.8321E-03	.1000E-01	.1656E-14	.1536E-14
.4	.8314E-03	.8337E-02	.8314E-03	.1000E-01	.3280E-14	.2815E-14
.5	.8305E-03	.8339E-02	.8305E-03	.1000E-01	.7039E-14	.5472E-14
.6	.8294E-03	.8341E-02	.8294E-03	.1000E-01	.1669E-13	.1164E-13
.7	.8281E-03	.8344E-02	.8281E-03	.1000E-01	.4311E-13	.2688E-13
.8	.8266E-03	.8347E-02	.8266E-03	.1000E-01	.1223E-12	.6834E-13
.9	.8248E-03	.8351E-02	.8248E-03	.1000E-01	.3864E-12	.1955E-12
1.0	.8226E-03	.8355E-02	.8226E-03	.1000E-01	.1380E-11	.6397E-12
1.1	.8199E-03	.8361E-02	.8199E-03	.1000E-01	.5706E-11	.2449E-11
1.2	.8161E-03	.8368E-02	.8161E-03	.1000E-01	.2820E-10	.1131E-10
1.3	.8108E-03	.8379E-02	.8108E-03	.1000E-01	.1746E-09	.6589E-10
1.4	.8027E-03	.8395E-02	.8027E-03	.1000E-01	.1452E-08	.5163E-09
1.5	.7893E-03	.8423E-02	.7893E-03	.1000E-01	.1811E-07	.6040E-08
1.6	.7646E-03	.8473E-02	.7646E-03	.1000E-01	.4108E-06	.1262E-06
1.7	.7110E-03	.8581E-02	.7110E-03	.1000E-01	.2487E-04	.6670E-05

Table for optimal β's, their row-sum and the square norm of local truncation error functionals in $L^2(C_r)$ space for Cowell's 3-points usual method and the corresponding optimal method interpolatory for $\exp(\pm1.6x)$, at the nodal points, with r=2.01, a=-1.8, b=1.8, n=36, h=.1; $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$; $\beta_0=.083333$, $\beta_1=.833333$, $\beta_2=.083333$.

Table - 7b

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	2	.244871E-03	2	.198267E-04
2	2	.610703E-04	2	.413152E-04
3	3	.430195E-03	2	.865679E-05
4	2	.133292E-03	2	.594996E-04
5	2	.348263E-03	2	.101422E-03
6	3	.127772E-03	2	.106507E-04
7	2	.313175E-04	2	.256370E-05
8	2	.133523E-03	2	.102367E-04
9	2	.735570E-04	2	.570366E-05
10	1	.111844E-02	1	.236393E-03
11	1	.575402E-03	1	.392509E-03
12	1	.555353E-03	1	.389258E-03
13	2	.174323E-05	2	.496382E-06
14	2	.103607E-05	1	.239882E-06
15	2	.224814E-05	2	.699675E-06
16	2	.142465E-05	2	.354305E-06
17	1	.146848E-07	1	.220510E-08
18	1	.920340E-07	1	.373346E-08
19	3	.509406E-03	2	.229013E-04
20	3	.464907E-03	2	.206231E-04
21	2	.304134E-03	2	.345624E-04
22	2	.208304E-03	2	.249211E-04
23	2	.300455E-03	2	.115582E-03
24	2	.287372E-04	2	.273774E-05

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for functions exp(±1.6x), in $L^2(C_r)$ space, for 24 BVP-s.

The results of Table 7b are obtained with r=2.01, a=-1.8, b=1.8, n=36, h=.1 for BVP's with equations 1-9 and 19-24 and with r=2.8, a=-2, b=2, n=40, h=.1 for BVP's with equations 10-18. Table 7b reveals that as compared to usual method, β-optimal method interpolatory for linearly independent functions exp(±1.6x) for BVP's is two decimal places better on equation 3; one decimal place better on equations 1,4,6-10,14-22,24; and just better on equations 2,5,11-13,23.

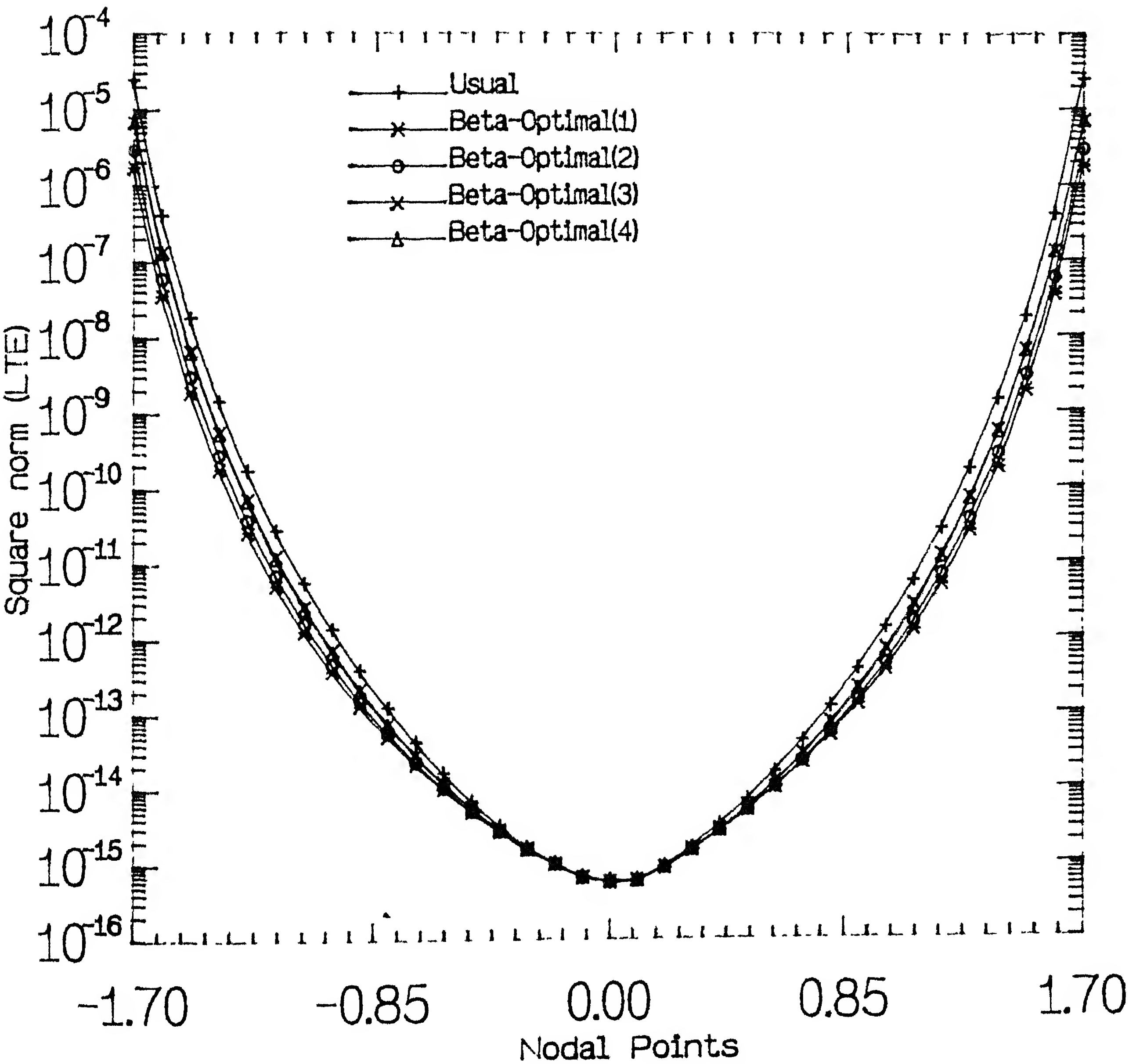
Table - 7c

eqn.	itu	$\bar{e}_u$	ito	$\bar{e}_o$
1	5	.140932E-01	4	.757542E-03
2	4	.250457E-02	4	.133628E-02
3	8	.760039E-01	4	.147005E-02
4	5	.132805E-01	4	.404481E-02
5	4	.716823E-02	4	.185820E-02
6	5	.356402E-02	4	.372113E-03
7	4	.354625E-03	3	.375720E-04
8	4	.211573E-02	3	.104763E-03
9	3	.604542E-03	3	.289515E-04
10	4	.119641E-01	4	.596451E-02
11	4	.130464E+00	3	.244210E-03
12	4	.129361E+00	3	.839701E-03
13	2	.128426E-05	2	.652674E-06
14	2	.831124E-06	2	.446034E-06
15	2	.193794E-05	2	.875456E-06
16	2	.130401E-05	2	.576796E-06
17	1	.456442E-08	1	.212508E-09
18	1	.343343E-07	1	.876228E-08
19	11	.103867E+00	5	.514932E-02
20	4	.188589E-02	3	.132981E-03
21	4	.112364E-02	3	.934208E-04
22	5	.115497E-01	4	.103295E-02
23	4	.610397E-02	4	.203661E-02
24	3	.542588E-04	2	.174337E-05

Table for number of iterations for convergence of the solution and the average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for functions exp(±1.6x), in $L^2(C_r)$ space, for 24 IVP-s.

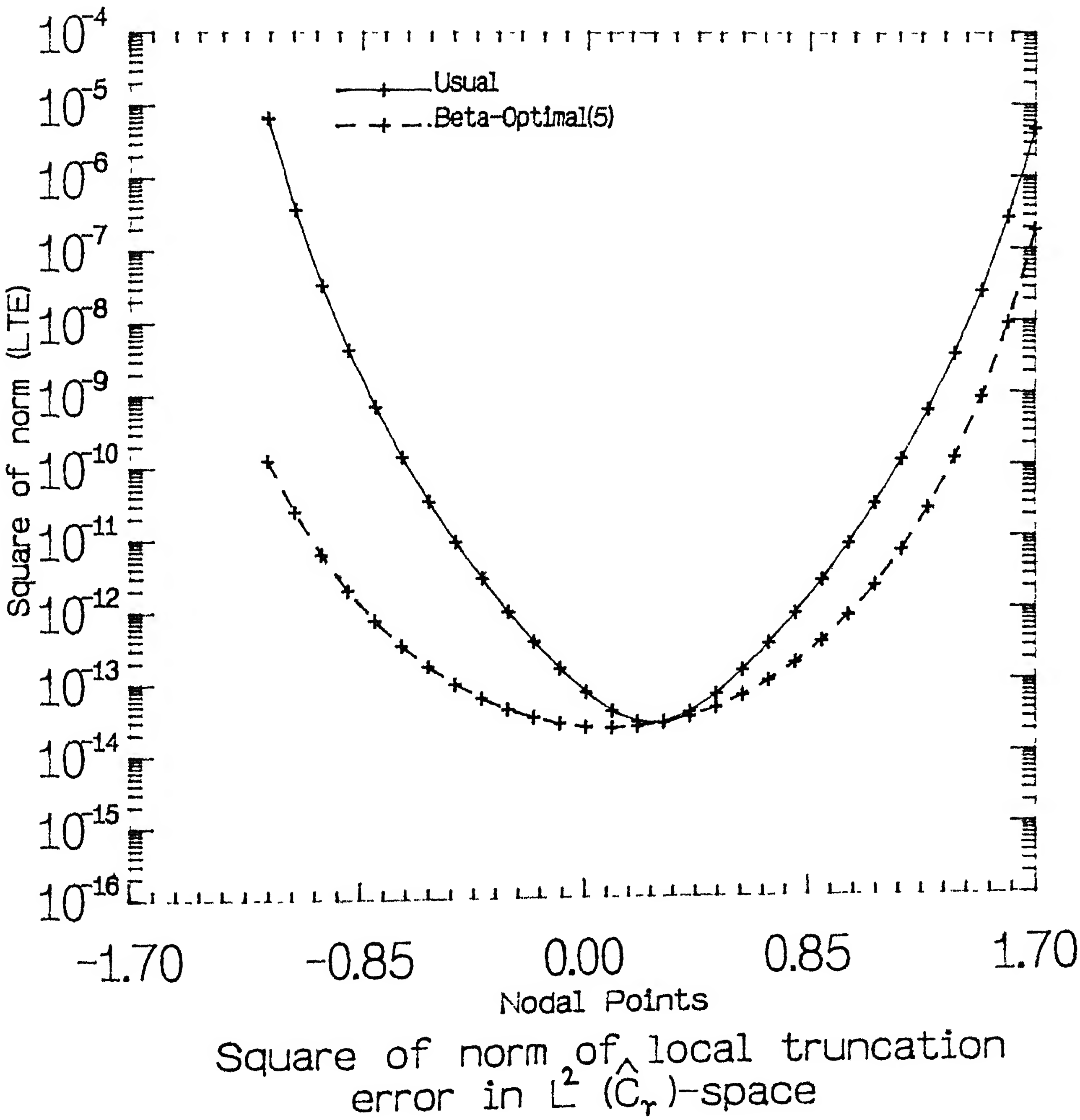
The results of Table 7c are obtained with r=2.01, a=-1.7, b=1.7, n=34, h=.1 for IVP's with equations 1-9 and 19-24 and with r=2.7, a=-1.4, b=1.4, n=28, h=.1 for IVP's with equations 10-18. Table 7c reveals that as compared to usual method β-optimal method interpolatory for linearly independent functions exp(±1.6x) for IVP is three decimal places better on equations 11,12; two decimal places better on equations 1,19,21; one decimal place better on equations 3,4,6-10,13,15-18,20,22 and 24; and just better on equations 2,5,14 and 23.

In Figure 1, we are showing the graphs for the square norm of local truncation error functionals for the usual Cowell's method with function evaluation at three points [Usual] and those for the corresponding β-optimal method [Beta-optimal(1)], β-optimal method with restriction [Beta-Optimal(2)], β-optimal method interpolatory for polynomials of degree 3 [Beta-optimal(3)] and β-optimal method iterpolatory for linearly independent functions $\exp(\pm 1.6x)$ [Beta-optimal(4)], with the numerical results given in the Tables 2a, 5a, 6a and 7a. From Figure 1, we see that, the curves for Beta-Optimal(2), Beta-Optimal(3), Beta-Optimal(4) lie in between the curves for Usual and Beta-Optimal(1). So, β-optimal method is giving more optimized results than other optimal methods. Figure 2 presents the graphs for the square norm of local truncation error functionals for the usual Stormer's method with function evaluation at five points [Usual] and that for the corresponding β-optimal method [Beta-optimal(5)]. Figure 3 presents the square norm of local truncation error functional for the usual Cowell's method with function evaluation at three points [Usual] and that for the corresponding α-optimal method. This figure reveals that α-optimal method is not giving so promising results.



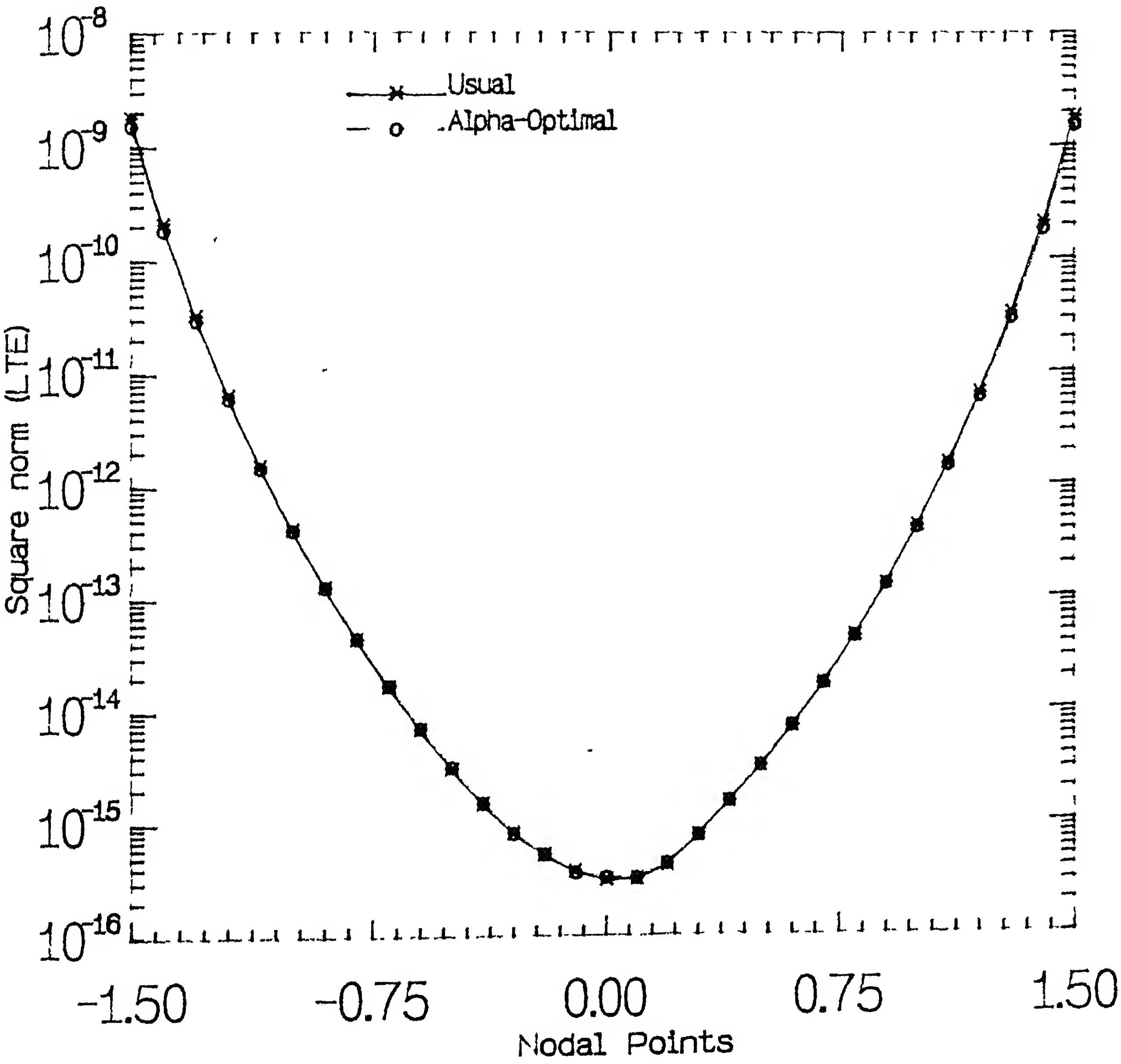
Square of norm of local truncation error in $L^2(\hat{C}_\gamma)$-space

FIG. 1



Usual
Beta-Optimal(5)
Square of norm (LTE)
10^{-4}
10^{-5}
10^{-6}
10^{-7}
10^{-8}
10^{-9}
10^{-10}
10^{-11}
10^{-12}
10^{-13}
10^{-14}
10^{-15}
10^{-16}
-1.70
-0.85
0.00
0.85
1.70
Nodal Points
Square of norm of local truncation error in $L^2(\hat{C}_r)$-space

FIG. 2



Square of norm of local truncation error in $L^2(\hat{C}_\gamma)$-space

FIG. 3

To obtain the coefficients $\hat{\alpha}^F_{j,n}$, $j = 0(1)k$ of an α-optimal multistep method

$$(15) \qquad \sum_{j=0}^{k} \hat{\alpha}^F_{j,n}\, y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j\, f_{n+k-j} = 0,$$

in $L^2(\hat{C}_r)$ space with prefixed β_j's, interpolatory for q number of linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$, we have to solve a system of linear equations given in the matrix form as

$$\begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} a \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where $A = (A_{ij})_{\substack{i=0(1)k,\\ j=0(1)k}}$ with $A_{ij} = \dfrac{r^2}{\pi(r^2 - x_{n+k-j}\bar{x}_{n+k-i})}$;

$F = (F_{ij})_{\substack{i=1(1)q,\\ j=0(1)k}}$ with $F_{ij} = f_i(x_{n+k-j})$;

$a = \left(\hat{\alpha}^F_{0,n}, \hat{\alpha}^F_{1,n}, \ldots, \hat{\alpha}^F_{k,n}\right)^T$; $\quad \lambda = (\lambda_1, \lambda_2, \ldots, \lambda_q)^T$;

$c = (c_0, c_1, \ldots, c_k)^T$, with $c_i = -h^2 \sum_{j=\delta_{t0}}^{k} \beta_j \dfrac{6r^2}{\pi} \dfrac{x^2_{n+k-i}}{(r^2 - x_{n+k-i}\bar{x}_{n+k-j})^3}$;

and

$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T$; $\quad$ with $\tilde{f}_i = -h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_i''(x_{n+k-j})$.

This method is characterized as follows.

<u>Theorem 10</u>: An α-optimal multistep method (15), in $L^2(\hat{C}_r)$ space interpolatory for arbitrary functions $f_1, f_2, \ldots, f_q$ is characterized by that it is locally interpolatory for the functions

$$\{ f_1, f_2, \ldots, f_q \} \cup \{ h_i,\ i = 0(1)k-q \},$$

where

$$h_i(x) = \frac{1}{(r^2-x\bar{x}_{n+k-i})^2} - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\,i+1} \frac{1}{(r^2-x\bar{x}_{n+k-j})^2},$$

and $\quad G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}}$, where

$$P = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=k-q+1(1)k}}, \quad \text{and} \quad E = \Big(f_i(x_{n+k-j})\Big)_{\substack{i=1(1)q \\ j=0(1)k-q}}.$$

Proof: The proof follows from Theorem 9 of Chapter 1.

5.6 Behavior of the Coefficients as $r \longrightarrow \infty$

In section 4.6, we have studied a limiting behavior, as $r \rightarrow \infty$, of the coefficients in the optimal multistep method in the space $H^2(C_r)$. Analogs of those results also remain valid for the space $L^2(\hat{C}_r)$ with the only change in the proofs that instead of the orthonormal basis $\{\psi_k\}$ for $H^2(C_r)$ space, here the orthonormal basis $\{\psi_k\}$ for $L^2(\hat{C}_r)$ space is required. So, in this section we just give the statements of the corresponding results in $L^2(\hat{C}_r)$ space and omit their proofs.

Theorem 11: Let

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j^F f_{n+k-j} = 0 \tag{16}$$

be a multistep method interpolatory for functions $\left\{\phi_{\delta_{t0}}, \ldots, \phi_k\right\}$ and let the matrix $[\phi_i''(x_{n+k-j})]_{i,j=\delta_{t0}(1)k}$ be nonsingular. Let

(17) $$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} f_{n+k-j} = 0$$

be an optimal multistep formula in $L^2(\hat{C}_r)$ space, interpolatory for functions $\left\{\phi_{\delta_{t0}}, \ldots, \phi_{p-1+\delta_{t0}}\right\}$, $0 \le p \le k + \delta_{t1} = k + 1 - \delta_{t0}$, where p=0 implies the non-interpolatory case for these functions. If the local truncation error functional $\hat{T}^F_{nr}$ for (17) satisfies

(18) $$\lim_{r \to \infty} \hat{T}^F_{nr}(\phi_j) = 0, \qquad j = p+\delta_{t0}(1)k$$

then

(19) $$\lim_{r \to \infty} \hat{\beta}^F_{j,r} = \beta^F_j \quad , \qquad j = \delta_{t0}(1)k$$

Theorem 12: Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k} \alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Then the $L^2(\hat{C}_r)$-coefficients $\hat{\beta}_{j,r}$ of an optimal multistep method

(20) $$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} f_{n+k-j} = 0$$

approach the coefficients β_j of the usual multistep method

(21) $$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0$$

of maximal polynomial precision.

Theorem 13: Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k} \alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Then the $L^2(\hat{C}_r)$-coefficients $\hat{\beta}^P_{j,r}$ of an optimal multistep method

$$(22) \qquad \sum_{j=0}^{k}\alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^P_{j,r} f_{n+k-j} = 0,$$

interpolatory for polynomials of degree $p \le k+\delta_{t1}+1$, approach, as $r \longrightarrow \infty$, the coefficients β_j of the corresponding usual multistep method

$$\sum_{j=0}^{k}\alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0.$$

<u>Theorem 14</u>: Let α_j, $j = 0(1)k$ be constants such that $\sum_{j=0}^{k}\alpha_j = 0$, and $\sum_{j=1}^{k} j\alpha_j = 0$. Let the $(k+\delta_{t1})\mathrm{x}(k+\delta_{t1})$ matrix M be nonsingular, where

$$M = \begin{bmatrix} \phi_1''(x_{n+k-1+\delta_{t1}}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots & \phi_1''(x_n) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & \\ \phi_p''(x_{n+k-1+\delta_{t1}}) \ldots\ldots\ldots\ldots\ldots\ldots\ldots & \phi_p''(x_n) \\ 1 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots 1 & \\ x_{n+k-1+\delta_{t1}} \ldots\ldots\ldots\ldots\ldots\ldots\ldots x_n & \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots & \\ x_{n+k-1+\delta_{t1}}^{k-p-\delta_{t0}} \ldots\ldots\ldots\ldots\ldots\ldots & x_n^{k-p-\delta_{t0}} \end{bmatrix}$$

Then the coefficients $\hat{\beta}^F_{k-j,r}$'s of the optimal multistep method in $L^2(\hat{C}_r)$ space

$$(23) \qquad \sum_{j=0}^{k}\alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,r} f_{n+k-j} = 0,$$

interpolatory for functions $\{\phi_1,\phi_2,\ldots,\phi_p\}$, $p \le k+\delta_{t1}$, approach the coefficients β^F_j 's of the unique multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} - h^2 \sum_{j=\delta_{t0}}^{k} \beta_j^F f_{n+k-j} = 0, \tag{24}$$

which is interpolatory for functions

$$\{\phi_1, \phi_2, \ldots, \phi_p, x^2, x^3, \ldots, x^{k+\delta_{t1}+1-p}\}.$$

CHAPTER - 6

OPTIMAL MULTISTEP METHODS IN $H_{a,b}^{(m)}$ SPACE

6.1 Introduction

Optimal quadrature rules in the Hilbert space $H_{0,1}^{(2)}$, have been studied by Larkin [126], where $H_{0,1}^{(2)}$ is the Hilbert space of real valued functions, of a real variable x, having square integrable second derivatives over the interval [0,1], with an inner product defined by:

$$(f(x),g(x)) = \alpha f(0)g(0) + \beta f'(0)g'(0) + \int_0^1 f''(y)g''(y)dy,$$

where α and β are positive real constants.

In this chapter, we define the Hilbert space $H_{a,b}^{(m)}$, to be the class of real valued functions, of a real variable x, having square integrable m-th derivatives over the interval [a,b], with an inner product defined by

$$(f(x),g(x)) = \sum_{i=0}^{m-1} c_i f^{(i)}(a)\; g^{(i)}(a) + \int_a^b f^{(m)}(y)\; g^{(m)}(y)dy,$$

where c_i, $i = 0(1)m-1$ are positive real constants.

In section 6.2, we obtain the reproducing kernel function for the Hilbert space $H_{a,b}^{(m)}$ and verify that the second derivative of this kernel is indeed the representer of the second derivative evaluation functional.

In this chapter, we discuss various optimal multistep methods, discussed in Chapter 1, in Hilbert spaces $H_{a,b}^{(m)}$ for $m \geq 3$. The methodology for convergence for β-optimal multistep method as given in Chapter 3 (Theorem 5 and 6) are valid in a Hilbert space, H, in

which D_x^{p+2}, the p+2-th derivative evaluation functional at x exists and is uniformly bounded on [a,b], where p is the order of the linear difference operator associated with the corresponding usual method. In $H_{a,b}^{(m)}$-space, D_x^{m-1}, the representer for the (m-1)-th derivative evaluation functional at x exists and is bounded on a closed subinterval of the interval [a,b]. As we know, p equals 2 for Stormer's usual method with function evaluation at one point and p equals 4 for Cowell's usual method with function evaluation at three points, the hypothesis of convergence are not satisfied for the functions in the spaces $H_{a,b}^{(m)}$ for m = 3 and 4 in case of Stormer's method and in the spaces $H_{a,b}^{(m)}$ for m = 3, 4, 5 and 6 in case of Cowell's method. But still the numerical results on these spaces suggest that optimal methods perform better than the corresponding usual method.

We discuss β-optimal multistep methods in the spaces $H_{a,b}^{(m)}$ and their numerical illustrations in section 6.3, β-optimal multistep methods interpolatory for polynomials of certain degree in the spaces $H_{a,b}^{(m)}$ and their numerical implementations in section 6.4, and β-optimal multistep methods interpolatory for linearly independent functions in the spaces $H_{a,b}^{(m)}$ and their numerical implementations in section 6.5.

We shall implement numerically various optimal methods viz., β-optimal method, β-optimal method with restriction, β-optimal method interpolatory for polynomials of certain degree, β-optimal method interpolatory for linearly independent functions, taking Cowell's method with function evaluation at three points and Stormer's method with function evaluation at one point as the usual

method, on the boundary value problems with differential equations of the form,
$$\frac{d^2y}{dx^2} = f(x,y),$$
whose true solutions are given as follows.

1. $y = |x - .5|^3,$
2. $y = |x - .5|^3 + |x + .5|^3,$
3. $y = |x - 1|^3 + |x + 1|^3,$
4. $y = |x - 1.5|^3 + |x + 1.5|^3,$
5. $y = |x - .5|^3 + |x - 1|^3 + |x - 1.5|^3,$
6. $y = |x - .6|^3,$
7. $y = |x - 1|^{2\,7},$
8. $y = |x - 1|^{2\,8},$
9. $y = |x - 1|^{2\,9},$
10. $y = |x - 1|^{3\,1}.$

With the true solution of the form $y = |x - a|^b$, we take the associated differential equation of the form
$$y'' = g(x) = b(b-1)|x - a|^{b-2}.$$

For the numerical implementation of β-optimal methods interpolatory for arbitrary functions and β-optimal methods corresponding to Stormer's one point method, we use different sets of differential equations.

In our numerical experiments corresponding to Cowell's and Stormer's usual methods, the optimal beta coefficients in a higher derivative space, such as $H^{(m)}_{a,b}$, $m \geq 6$, turn out to be nearly equal to the corresponding usual coefficients and consequently both the methods produce almost equal numerical results including some round off errors. So, for numerical implementation, we are interested in

a lower derivative space such as $H^{(m)}_{a,b}$, m=3,4,5. For the numerical experimentation in space $H^{(m)}_{a,b}$, we take the parameters c_i's as 1. We use the notations in the tables as 'r-sum' for the row sum of $\hat{\beta}_{i,n}$, i=1,2,3, $\|T_n\|^2$ and $\|\hat{T}_n\|^2$ for the square norm of local truncation error functionals for usual and β-optimal methods respectively, $\bar{e}_u$ and $\bar{e}_0$ for the average of absolute discretization errors for usual and β-optimal methods respectively.

6.2 Derivation of Kernel and the Representer of the Second Derivative Evaluation Functional.

The reproducing kernel function for the Hilbert space $H^{(m)}_{a,b}$ ought to satisfy the relation

$$(1)\quad f(x)=(f(y),K(y,x))=\sum_{i=0}^{m-1} c_i f^{(i)}(a)K^{(i)}(a,x)+\int_a^b f^{(m)}(y)K^{(m)}(y,x)\,dy.$$

Now, on integration by parts,

$$\int f^{(m)}(y)K^{(m)}(y,x)\,dy = \sum_{i=0}^{m-1}(-1)^i K^{(m+i)}(y,x)f^{(m-i-1)}(y) + (-1)^m\int K^{(2m)}(y,x)f(y)\,dy.$$

Hence,

$$\int_a^b f^{(m)}(y)\quad K^{(m)}(y,x)\,dy = \sum_{i=0}^{m-1}(-1)^i K^{(m+i)}(y,x)f^{(m-i-1)}(y)\Big|_a^b - \sum_{i=0}^{m-1}(-1)^i K^{(m+i)}(y,x)f^{(m-i-1)}(y)\Big|_{x^-}^{x^+} + (-1)^m\int_a^b K^{(2m)}(y,x)f(y)\,dy$$

$$= \sum_{i=0}^{m-1}(-1)^i K^{(m+i)}(b,x)f^{(m-i-1)}(b) - \sum_{i=0}^{m-1}(-1)^i K^{(m+i)}(a,x)f^{(m-i-1)}(a)$$

$$- \sum_{i=0}^{m-1} (-1)^i f^{(m-i-1)}(x) \left[K^{(m+i)}(x^+,x) - K^{(m+i)}(x^-,x)\right]$$

$$+ (-1)^m \int_a^b K^{(2m)}(y,x) f(y) dy.$$

So, from (1),

$$f(x) = \sum_{i=0}^{m-1} c_i f^{(i)}(a) \; K^{(i)}(a,x) + \sum_{i=0}^{m-1} (-1)^i K^{(m+i)}(b,x) f^{(m-i-1)}(b)$$

$$- \sum_{i=0}^{m-1} (-1)^{m-i-1} K^{(2m-i-1)}(a,x) f^{(i)}(a)$$

$$- \sum_{i=0}^{m-1} (-1)^{m-i-1} f^{(i)}(x) \left[K^{(2m-i-1)}(x^+,x) - K^{(2m-i-1)}(x^-,x)\right]$$

$$+ (-1)^m \int_a^b K^{(2m)}(y,x) f(y) dy$$

$$= \sum_{i=0}^{m-1} f^{(i)}(a) \left[c_i K^{(i)}(a,x) + (-1)^{m-i} K^{(2m-i-1)}(a,x)\right]$$

$$+ \sum_{i=0}^{m-1} (-1)^i K^{(m+i)}(b,x) f^{(m-i-1)}(b)$$

$$- \sum_{i=0}^{m-1} (-1)^{m-i-1} f^{(i)}(x) \left[K^{(2m-i-1)}(x^+,x) - K^{(2m-i-1)}(x^-,x)\right]$$

$$+ (-1)^m \int_a^b K^{(2m)}(y,x) f(y) dy.$$

Comparing both sides we get the following equations:

(2) $$c_i K^{(i)}(a,x) + (-1)^{m-i} K^{(2m-i-1)}(a,x) = 0, \quad i = 0(1)m-1,$$

(3) $$K^{(m+i)}(b,x) = 0 \;, \quad i = 0(1)m-1,$$

(4) $$K^{(2m-i-1)}(x^+,x) - K^{(2m-i-1)}(x^-,x) = 0, \quad i = 1(1)m-1,$$

(5) $$(-1)^{m-1} \left[K^{(2m-1)}(x^-,x) - K^{(2m-1)}(x^+,x)\right] = 1,$$

(6) $$K^{(2m)}(y,x) = 0,$$

also by continuity of the kernel $K(y,x)$ at x, we have

(7) $$K^{(i)}(x^+,x) = K^{(i)}(x^-,x), \qquad i = 0(1)m-1.$$

By (6), we have

$$K(y,x) = \begin{cases} \sum_{j=0}^{2m-1} \tilde{\beta}_j\, y^j, & a \le y \le x \\ \sum_{j=0}^{2m-1} \tilde{\gamma}_j\, y^j, & x \le y \le b \end{cases}$$

Setting $y = a + (b-a)t$ and $x = a + (b-a)s$, where $0 \le s,t \le 1$, we can write

$$K(y,x) = K_1(t,s) = \begin{cases} \sum_{j=0}^{2m-1} \beta_j\, t^j, & 0 \le t \le s \\ \sum_{j=0}^{2m-1} \gamma_j\, t^j, & s \le t \le 1 \end{cases}$$

or,

(8) $$K(y,x) = K_1(t,s) = \begin{cases} \sum_{j=0}^{2m-1} \beta_j \left(\frac{y-a}{b-a}\right)^j, & 0 \le \frac{y-a}{b-a} \le \frac{x-a}{b-a} \\ \sum_{j=0}^{2m-1} \gamma_j \left(\frac{y-a}{b-a}\right)^j, & \frac{x-a}{b-a} \le \frac{y-a}{b-a} \le 1 \end{cases}$$

$$K^{(i)}(y,x) = \frac{1}{(b-a)^i} K_1^{(i)}(t,s)$$

By (2), we have, for $i = 0(1)m-1$

$$c_i \frac{1}{(b-a)^i} \beta_i\, i! + (-1)^{m-i} \frac{1}{(b-a)^{2m-i-1}} \beta_{2m-i-1} (2m-i-1)! = 0.$$

So, $$\beta_{2m-i-1} = (-1)^{m-i-1} (b-a)^{2m-2i-1} \frac{c_i\, i!}{(2m-i-1)!} \beta_i, \qquad i = 0(1)m-1.$$

By (3), we have

$$\gamma_{m+i}\frac{(m+i)!}{(b-a)^{m+i}}+\frac{\gamma_{m+i+1}}{(b-a)^{m+i}}\frac{(m+i+1)!}{1!}+\frac{\gamma_{m+i+2}}{(b-a)^{m+i}}\frac{(m+i+2)!}{2!}+\cdots\cdots$$

$$+\frac{\gamma_{2m-1}}{(b-a)^{m+i}}\frac{(2m-1)!}{(m-i-1)!}=0,\quad i=0(1)m-1.$$

So, $\gamma_m=\gamma_{m+1}=\cdots\cdots=\gamma_{2m-1}=0$.

By (8), $K(y,x)$ can be written as

$$\text{(9)}\quad K(y,x)=\begin{cases}\displaystyle\sum_{j=0}^{m-1}\beta_j\left[\left(\frac{y-a}{b-a}\right)^j+\frac{(-1)^{m-j-1}(b-a)^{2m-2j-1}c_j j!}{(2m-j-1)!}\left(\frac{y-a}{b-a}\right)^{2m-j-1}\right], & \\ \qquad\qquad \text{for} \quad 0\le\frac{y-a}{b-a}\le\frac{x-a}{b-a} & \\ \displaystyle\sum_{j=0}^{m-1}\gamma_j\left(\frac{y-a}{b-a}\right)^j, \qquad \text{for} \quad \frac{x-a}{b-a}\le\frac{y-a}{b-a}\le 1. & \end{cases}$$

By (5), we have

$$(-1)^{m-1}(-1)^{m-1}\;\beta_0\frac{(b-a)^{2m-1}c_0}{(2m-1)!}\frac{(2m-1)!}{(b-a)^{2m-1}}=1.$$

So,

$$\text{(10)}\qquad \beta_0=\frac{1}{c_0}.$$

Since $K^{(2m-i-1)}(x^+,x)=0$, for $i=1(1)m-1$, we have, from (4)

$$\text{(11)}\qquad K^{(2m-2)}(x^-,x)=K^{(2m-3)}(x^-,x)=\cdots\cdots\cdots=K^{(m)}(x^-,x).$$

Now, $K^{(2m-2)}(x^-,x)=0$, gives

$$\beta_0\frac{(-1)^{m-1}(b-a)^{2m-1}c_0}{(2m-1)!}\frac{(2m-1)!}{1!(b-a)^{2m-2}}\frac{x-a}{b-a}+$$

$$\beta_1\frac{(-1)^{m-2}(b-a)^{2m-3}c_1 1!}{(2m-2)!}\frac{(2m-2)!}{(b-a)^{2m-2}}=0.$$

Using (10), we get

$$\text{(12)}\qquad \beta_1=(b-a)^2\frac{1}{c_1}\frac{x-a}{b-a}.$$

Further $K^{(2m-3)}(x^-,x) = 0$, gives

$$\beta_0 \frac{(-1)^{m-1}(b-a)^{2m-1}c_0 0!}{(2m-1)!} \frac{(2m-1)!}{2!(b-a)^{2m-3}} \left(\frac{x-a}{b-a}\right)^2 +$$

$$+ \beta_1 \frac{(-1)^{m-2}(b-a)^{2m-3}c_1 1!}{(2m-2)!} \frac{(2m-2)!}{(b-a)^{2m-3}} \frac{x-a}{b-a} +$$

$$+ \beta_2 \frac{(-1)^{m-3}(b-a)^{2m-5}c_2 2!}{(2m-3)!} \frac{(2m-3)!}{(b-a)^{2m-3}} = 0.$$

Using (10) and (12), we get

(13) $$\beta_2 = \frac{(b-a)^4}{2!2!c_2} \left(\frac{x-a}{b-a}\right)^2.$$

Let us assume that

(14) $$\beta_i = \frac{1}{i!i!} \frac{(b-a)^{2i}}{c_i} \left(\frac{x-a}{b-a}\right)^i; \qquad \text{for all } i = 0(1)j.$$

Now $K^{(2m-j-2)}(x^-,x) = 0$, from (11), gives:

$$\beta_{j+1}c_{j+1}(-1)^{m-j-2} \frac{(b-a)^{2m-2j-3}}{(2m-j-2)!} \frac{(j+1)!(2m-j-2)!}{0!} +$$

$$\beta_j c_j (-1)^{m-j-1} \frac{(b-a)^{2m-2j-1}}{(2m-j-1)!} \frac{j!(2m-j-1)!}{1!} \left(\frac{x-a}{b-a}\right) +$$

$$\beta_{j-1}c_{j-1}(-1)^{m-j} \frac{(b-a)^{2m-2j+1}}{(2m-j)!} \frac{(j-1)!(2m-j)!}{2!} \left(\frac{x-a}{b-a}\right)^2 + \ldots\ldots +$$

$$\beta_1 c_1 (-1)^{m-2} \frac{(b-a)^{2m-3}}{(2m-2)!} \frac{1!(2m-2)!}{j!} \left(\frac{x-a}{b-a}\right)^j +$$

$$\beta_0 c_0 (-1)^{m-1} \frac{(b-a)^{2m-1}}{(2m-1)!} \frac{0!(2m-1)!}{(j+1)!} \left(\frac{x-a}{b-a}\right)^{j+1} = 0.$$

Substituting the values of β_i, $i = 0(1)j$, we get

$$\beta_{j+1}c_{j+1}(-1)^{m-j-2}(b-a)^{2m-2j-3}(j+1)! \quad + \quad (-1)^{m-j-1}\frac{(b-a)^{2m-1}}{1!j!} \left(\frac{x-a}{b-a}\right)^{j+1} +$$

$$(-1)^{m-j}\frac{(b-a)^{2m-1}}{2!(j-1)!}\left(\frac{x-a}{b-a}\right)^{j+1} + (-1)^{m-j+1}\frac{(b-a)^{2m-1}}{3!(j-2)!}\left(\frac{x-a}{b-a}\right)^{j+1} + \cdots\cdots$$

$$+(-1)^{m-2}\frac{(b-a)^{2m-1}}{j!1!}\left(\frac{x-a}{b-a}\right)^{j+1} + (-1)^{m-1}\frac{(b-a)^{2m-1}}{(j+1)!}\left(\frac{x-a}{b-a}\right)^{j+1} = 0.$$

Cancelling $(-1)^m(b-a)^{2m-1}$ throughout we get

$$(-1)^{-j-2}\beta_{j+1}c_{j+1} = \frac{1}{(j+1)!}(b-a)^{2(j+1)}\left(\frac{x-a}{b-a}\right)^{j+1}$$

$$\cdot\left[\frac{1}{(j+1)!} - \frac{1}{j!1!} + \frac{1}{(j-1)!2!} - \cdots + \frac{(-1)^{-j+2}}{3!(j-2)!} + \frac{(-1)^{-j+1}}{2!(j-1)!} + \frac{(-1)^{-j}}{1!j!}\right]$$

$$= \frac{1}{(j+1)!}(b-a)^{2(j+1)}\left(\frac{x-a}{b-a}\right)^{j+1}$$

$$\cdot\left[\frac{1}{(j+1)!} - \frac{1}{j!1!} + \frac{1}{(j-1)!2!} - \cdots + \frac{(-1)^{j-2}}{3!(j-2)!} + \frac{(-1)^{j-1}}{2!(j-1)!} + \frac{(-1)^{j}}{1!j!}\right].$$

We know,

$$0 = (1-1)^{j+1} = 1 - {}^{j+1}C_1 + {}^{j+1}C_2 - \cdots\cdots + (-1)^j\,{}^{j+1}C_j + (-1)^{j+1}\,{}^{j+1}C_{j+1}.$$

So,

$$\frac{1}{(j+1)!} - \frac{1}{j!1!} + \frac{1}{(j-1)!2!} - \cdots + \frac{(-1)^{j-1}}{2!(j-1)!} + \frac{(-1)^{j}}{1!j!} = \frac{(-1)^{j+2}}{(j+1)!}.$$

Hence,

$$(15)\qquad \beta_{j+1}c_{j+1} = \frac{1}{[(j+1)!]^2}(b-a)^{2(j+1)}\left(\frac{x-a}{b-a}\right)^{j+1}.$$

By (10), (12), (13), (14) and (15) the induction follows. Thus

$$(16)\qquad \beta_i = \frac{1}{i!i!}\,\frac{(b-a)^{2i}}{c_i}\left(\frac{x-a}{b-a}\right)^{i}; \qquad \text{for all } i = 0(1)m-1$$

Substituting the values of β_i, $i = 0(1)m-1$, in (9), and writing $t = \frac{y-a}{b-a}$ and $s = \frac{x-a}{b-a}$, we get

$$K(y,x) = \begin{cases} \dfrac{1}{c_0}\left[1+\dfrac{(-1)^{m-1}(b-a)^{2m-1}c_0}{(2m-1)!}t^{2m-1}\right] + \\ \displaystyle\sum_{j=1}^{m-1} \dfrac{s^j(b-a)^{2j}}{j!j!c_j}\left[t^j + \dfrac{(-1)^{m-j-1}(b-a)^{2m-2j-1}c_j j!}{(2m-j-1)!}t^{2m-j-1}\right], \\ \qquad\qquad \text{for } 0 \le t \le s, \\ \displaystyle\sum_{j=0}^{m-1} \gamma_j t^j, \qquad\qquad \text{for } s \le t \le 1. \end{cases}$$

As $f(x) = (f(t),K(t,x))$, we have

$$(K(t,s),K(t,x)) = K(x,s).$$

Again in a real Hilbert space, inner product being symmetric, we have

$$(K(t,s),K(t,x)) = (K(t,x),K(t,s)) = K(s,x).$$

Thus, $K(x,s) = K(s,x)$. Hence, we can write

$$(17)\quad K(y,x) = \begin{cases} \dfrac{1}{c_0}\left[1 + \dfrac{(-1)^{m-1}(b-a)^{2m-1}c_0}{(2m-1)!}t^{2m-1}\right] + \\ \displaystyle\sum_{j=1}^{m-1} \dfrac{s^j(b-a)^{2j}}{j!j!c_j}\left[t^j + \dfrac{(-1)^{m-j-1}(b-a)^{2m-2j-1}c_j j!}{(2m-j-1)!}t^{2m-j-1}\right], \\ \qquad\qquad \text{for } 0 \le t \le s \\ \dfrac{1}{c_0}\left[1 + \dfrac{(-1)^{m-1}(b-a)^{2m-1}c_0}{(2m-1)!}s^{2m-1}\right] + \\ \displaystyle\sum_{j=1}^{m-1} \dfrac{t^j(b-a)^{2j}}{j!j!c_j}\left[s^j + \dfrac{(-1)^{m-j-1}(b-a)^{2m-2j-1}c_j j!}{(2m-j-1)!}s^{2m-j-1}\right], \\ \qquad\qquad \text{for } s \le t \le 1 \end{cases}$$

$$D2(y,x) = \frac{\partial^2}{\partial x^2} K(y,x)\Big|_x .$$

$$
\text{(18)}\quad D2(y,x)=\begin{cases}
\displaystyle\sum_{j=2}^{m-1}\frac{(-1)^{m-j-1}(b-a)^{2m-3}s^{j-2}t^{2m-j-1}}{(j-2)!(2m-j-1)!}+\sum_{j=2}^{m-1}\frac{(b-a)^{2j-2}s^{j-2}t^{j}}{(j-2)!j!c_j} & \text{for } 0\le t\le s\\[2ex]
\displaystyle\frac{(-1)^{m-1}(b-a)^{2m-3}s^{2m-3}}{(2m-3)!}+\sum_{j=1}^{m-1}\frac{(-1)^{m-j-1}(b-a)^{2m-3}s^{2m-j-3}t^{j}}{j!(2m-j-3)!}+ & \\
\displaystyle\qquad\sum_{j=2}^{m-1}\frac{(b-a)^{2j-2}s^{j-2}t^{j}}{(j-2)!j!c_j}, & \text{for } s\le t\le 1
\end{cases}
$$

For $i = 1(1)m-1$, we have

$$
D2^{(i)}(y,x) = \frac{\partial^2}{\partial y^2}\, D2(y,x)\Big|_x .
$$

$$
\text{(19)}\quad D2^{(i)}(y,x)=\begin{cases}
\displaystyle\sum_{j=2}^{m-1}\frac{(-1)^{m-j-1}(b-a)^{2m-3-i}s^{j-2}t^{2m-j-1-i}}{(j-2)!(2m-j-1-i)!}+ & \\
\displaystyle\qquad\sum_{j=i}^{m-1}\frac{(b-a)^{2j-2-i}s^{j-2}t^{j-i}}{(j-2)!(j-i)!c_j}, & \text{for } 0\le t\le s,\\[2ex]
\displaystyle\sum_{j=i}^{m-1}\frac{(-1)^{m-j-1}(b-a)^{2m-3-i}s^{2m-j-3}t^{j-i}}{(j-i)!(2m-j-3)!}+ & \\
\displaystyle\qquad\sum_{j=i}^{m-1}\frac{(b-a)^{2j-2-i}s^{j-2}t^{j-i}}{(j-2)!(j-i)!c_j}, & \text{for } s\le t\le 1.
\end{cases}
$$

Now for the space $H^{(m)}_{a,b}$, we directly verify, in the following theorem, that $D2(y,x)$, given by the second derivative of the kernel $K(y,x)$ is indeed the representer of the second derivative evaluation functional.

Theorem 1: The function $D2(y,x)$ given by (18) is the representer for the second derivative evaluation functional in $H^{(m)}_{2,c}$ space.

Proof: The m-th derivative of $D2(y,x)$ is given by

$$D2^{(m)}(y,x) = \frac{1}{(b-a)^{m+2}} \begin{cases} \sum_{j=2}^{m-1} \frac{(-1)^{m-j-1}(b-a)^{2m-1} s^{j-2} t^{m-j-1}}{(j-2)!(m-j-1)!}, & \text{for } 0 \le t \le s, \\ 0, & \text{for } s \le t \le 1. \end{cases}$$

$D2^{(m)}(y,x)$ is square integrable. So, $D2(y,x) \in H^{(m)}_{a,b}$. To complete the proof, we need to show that $f''(z_0) = (f(t), D2(t,z_0))$, for any point $z_0 \in [a,b]$. By (19), we have

$$D2(a\ ,\ z_0) = 0; \quad D2'(a,z_0) = 0,$$

$$D2^{(i)}(a\ ,\ z_0) = \frac{(b-a)^{i-2} s^{i-2}}{(i-2)!\,c_i}, \quad i=2(1)m-1$$

By the definition of the inner product of the space $H^{(m)}_{2,c}$, we have,

$(f(t), D2(t,z_0))$

$$= \sum_{i=0}^{m-1} c_i f^{(i)}(a) D2^{(i)}(a,z_0) + \int_a^b f^{(m)}(x) D2^{(m)}(x,z_0)\,dx$$

$$= \sum_{i=2}^{m-1} c_i f^{(i)}(a) \frac{(z_0-a)^{i-2}}{(i-2)!\,c_i} - \int_a^{z_0} \sum_{j=2}^{m-1} (-1)^{m-j-1} \frac{(z_0-a)^{j-2}(x-a)^{m-j-1}}{(j-2)!(m-j-1)!} f^{(m)}(x)\,dx.$$

Integrating by parts, we get

$(f(t), D2(t,z_0)) =$

$$(z_0-a)^{m-3} f^{(m-1)}(z_0) \left\{ \frac{1}{(m-3)!} - \frac{1}{(m-4)!1!} + \frac{1}{(m-5)!2!} - \ldots + \frac{(-1)^{m-3}}{(m-3)!} \right\}$$

$$+ (z_0-a)^{m-4} f^{(m-2)}(z_0) \left\{ \frac{1}{(m-4)!} - \frac{1}{(m-5)!1!} + \frac{1}{(m-6)!2!} - \ldots + \frac{(-1)^{m-4}}{(m-4)!} \right\}$$

$$+ \ldots\ldots\ldots\ldots + (z_0-a) f^{(3)}(z_0)\{1-1\} + f''(z_0).$$

Using the fact that

$$\frac{1}{j!} - \frac{1}{(j-1)!1!} + \frac{1}{(j-2)!2!} - \ldots + \frac{(-1)^{j-1}}{1!(j-1)!} + \frac{(-1)^j}{j!} = 0,$$

we get $(f(t), D2(t,z_0)) = f''(z_0)$. Hence the proof.

6.3 Optimal Multistep Methods in $H^{(m)}_{a,b}$ Space

In $H^{(m)}_{a,b}$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{t0}(1)k$ of β-optimal multistep method

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} f_{n+k-j} = 0, \tag{20}$$

where α_j's are prefixed according to some consistent and stable known usual method with highest degree polynomial precision,

$$\sum_{j=0}^{k} \alpha_j y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \beta_j f_{n+k-j} = 0. \tag{21}$$

With reference to equation (11) of Chapter 1, we have the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where

$$\hat{b} = h^2\left(\hat{\beta}_{\delta_{t0},n}, \ldots\ldots, \hat{\beta}_{k,n}\right)^T,$$

$\hat{c}_{ij}$, for $i, j = \delta_{t0}(1)k$, and $\hat{d}_i = -\sum_{j=0}^{k} \alpha_j \hat{d}_{ij}$, for $i = \delta_{t0}(1)k$ are defined as follows.

$$\hat{c}_{ij} = \begin{cases} \displaystyle\sum_{j=2}^{m-1} \frac{(-1)^{m-j-1}(x_{n+k-j}-a)^{2m-j-3}(x_{n+k-i}-a)^{j-2}}{(j-2)!(2m-j-3)!} + \\ \qquad \displaystyle\sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}(x_{n+k-j}-a)^{j-2}}{(j-2)!(j-2)!c_j}; \text{ for } x_{n+k-j} \le x_{n+k-i} \\ \displaystyle\sum_{j=2}^{m-1} \frac{(-1)^{m-j-1}(x_{n+k-i}-a)^{2m-j-3}(x_{n+k-j}-a)^{j-2}}{(j-2)!(2m-j-3)!} + \\ \qquad \displaystyle\sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}(x_{n+k-j}-a)^{j-2}}{(j-2)!(j-2)!c_j}; \text{ for } x_{n+k-j} \ge x_{n+k-i}. \end{cases}$$

and

$$\hat{d}_{ij} = \begin{cases} \displaystyle\sum_{j=2}^{m-1} \frac{(-1)^{m-j-1}(x_{n+k-j}-a)^{2m-j-1}(x_{n+k-i}-a)^{j-2}}{(j-2)!(2m-j-1)!} + \\ \qquad \displaystyle\sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}(x_{n+k-j}-a)^{j}}{(j-2)!j!c_j}; \text{ for } x_{n+k-j} \le x_{n+k-i} \\ \displaystyle\frac{(-1)^{m-1}(x_{n+k-i}-a)^{2m-3}}{(2m-3)!} + \sum_{j=1}^{m-1} \frac{(-1)^{m-j-1}(x_{n+k-i}-a)^{2m-j-3}(x_{n+k-j}-a)^{j}}{j!(2m-j-3)!} + \\ \qquad \displaystyle\sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}(x_{n+k-j}-a)^{j}}{(j-2)!j!c_j}; \text{ for } x_{n+k-j} \ge x_{n+k-i}. \end{cases}$$

This system of equations may be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{t0}(1)k$.

The following theorem characterizes the β-optimal multistep method (20) in $H^{(m)}_{a,b}$ space.

<u>Theorem 2:</u> The optimal multistep method (20) in which α_j's are prefixed, and optimization is done with respect to β_j's, in $H^{(m)}_{a,b}$ space, is characterized by that it is locally interpolatory for

functions $y_i(x)$, $i = \delta_{t0}(1)k$ where

$$
y_i(x) = \begin{cases}
\displaystyle\sum_{j=2}^{m-1} \frac{(-1)^{m-j-1}x^{2m-j-1}(x_{n+k-i}-a)^{j-2}}{(j-2)!(2m-j-1)!} + \sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}x^j}{(j-2)!j!c}, \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{for } x \le x_{n+k-i} \\
\displaystyle\frac{(-1)^{m-1}(x_{n+k-i}-a)^{2m-3}}{(2m-3)!} + \sum_{j=1}^{m-1} \frac{(-1)^{m-j-1}(x_{n+k-i}-a)^{2m-j-3}x^j}{j!(2m-j-3)!} + \\
\qquad\qquad\qquad \displaystyle\sum_{j=2}^{m-1} \frac{(x_{n+k-i}-a)^{j-2}x^j}{(j-2)!j!c_j} \quad \text{for } x \ge x_{n+k-i}.
\end{cases}
$$

Proof: The proof follows from Theorem 1 of Chapter 1, using the definitions of $K(z,\bar{t})$, $D2(t,\bar{z})$, $D2''(t,\bar{z})$ from (17), (18), (19).

The numerical results suggest that in space $H^{(m)}_{a,b}$, optimal beta coefficients $\hat{\beta}_{0n}$, $\hat{\beta}_{1n}$, $\hat{\beta}_{2n}$ for β-optimal method and the square norm of local truncation errors functionals for Cowell's usual and the corresponding β-optimal methods are independent of nodal points and the results for h=.1. are given as follows

$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
.1667E-02	.6667E-02	.1667E-02	.1000E-01	.5833E-06	.4444E-06

It seems that, $\hat{\beta}_{0n}=1/6$, $\hat{\beta}_{1n}=2/3$, $\hat{\beta}_{2n}=1/6$.

In the following table we present the numerical results for Cowell's usual and the corresponding β-optimal methods on the equations listed above on interval [-2, 2] for h = .1.

Table - 1(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.107441E-13
2	.961538E-02	.290665E-13
3	.769231E-02	.487416E-13
4	.448718E-02	.848324E-13
5	.108974E-01	.497921E-13
6	.466667E-02	.796221E-14
7	.102985E-01	.841119E-02
8	.749346E-02	.507054E-02
9	.539873E-02	.232991E-02
10	.270475E-02	.207524E-02

Table for average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method in $H^{(3)}_{a,b}$-space, for 10 BVP-s, with a=-2, b=2, n=40, h=.1.

The above numerical results show that as compared to usual method, the β-optimal method in $H^{(3)}_{a,b}$-space, with a=-2, b=2, n=40, h=.1, is far superior for BVP's with equations 1-6, one decimal place better for BVP's with equation 7 and just better on equations 8,9,10. If the function of the differential equation considered is not very smooth, then the optimal method is better suggested and if the function is smooth enough, then the usual method is better suggested. If the function is very bad, i.e., too far from smoothness then neither usual nor optimal method will perform better. This situation hold for β-optimization in $H^{(4)}_{a,b}$, $H^{(5)}_{a,b}$-space which are seen from the following tables.

Table - 2

	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.9	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-1.8	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.7	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.6	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.5	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.4	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.3	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.2	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.1	.1010E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.0	.1010E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-.9	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.8	.1011E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.7	.1011E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.6	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.5	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.4	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.3	.1012E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-.2	.1012E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
-.1	.1012E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.0	.1012E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.1	.1012E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.2	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.3	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.4	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1262E-09
.5	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
.6	.1011E-02	.7987E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
.7	.1011E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
.8	.1011E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
.9	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
1.0	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
1.1	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1454E-09	.1262E-09
1.2	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1454E-09	.1262E-09
1.3	.1010E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
1.4	.1010E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
1.5	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1456E-09	.1264E-09
1.6	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1456E-09	.1265E-09
1.7	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1457E-09	.1266E-09
1.8	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1457E-09	.1266E-09
1.9	.1009E-02	.7990E-02	.1002E-02	.1000E-01	.1458E-09	.1267E-09

Table for optimal β's, their row-sum and the square norm of local truncation error functionals for Cowell's 3-points usual and the corresponding β-optimal method in $H^{(4)}_{a,b}$ space, at the nodal points, with $a=-2$, $b=2$, $n=40$, $h=.1$, $\alpha_0=-1$ $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=.0833333$, $\beta_1=.833333$, $\beta_2=.0833333$.

Table - 3

	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\Vert T_n \Vert^2$	$\Vert \hat{T}_n \Vert^2$
-1.9	.8363E-03	.8327E-02	.8363E-03	.1000E-01	.8830E-13	.8736E-13
-1.8	.8361E-03	.8328E-02	.8361E-03	.1000E-01	.8795E-13	.8708E-13
-1.7	.8360E-03	.8328E-02	.8360E-03	.1000E-01	.8759E-13	.8676E-13
-1.6	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.8816E-13	.8734E-13
-1.5	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.8860E-13	.8779E-13
-1.4	.8361E-03	.8328E-02	.8360E-03	.1000E-01	.8861E-13	.8777E-13
-1.3	.8363E-03	.8328E-02	.8361E-03	.1000E-01	.8776E-13	.8690E-13
-1.2	.8364E-03	.8327E-02	.8362E-03	.1000E-01	.8804E-13	.8714E-13
-1.1	.8366E-03	.8327E-02	.8364E-03	.1000E-01	.8808E-13	.8713E-13
-1.0	.8368E-03	.8327E-02	.8366E-03	.1000E-01	.8705E-13	.8604E-13
-.9	.8371E-03	.8326E-02	.8368E-03	.1000E-01	.8773E-13	.8666E-13
-.8	.8373E-03	.8326E-02	.8370E-03	.1000E-01	.9176E-13	.9061E-13
-.7	.8376E-03	.8325E-02	.8372E-03	.1000E-01	.9188E-13	.9067E-13
-.6	.8378E-03	.8325E-02	.8374E-03	.1000E-01	.8998E-13	.8870E-13
-.5	.8380E-03	.8324E-02	.8376E-03	.1000E-01	.9181E-13	.9047E-13
-.4	.8382E-03	.8324E-02	.8378E-03	.1000E-01	.8925E-13	.8785E-13
-.3	.8384E-03	.8324E-02	.8379E-03	.1000E-01	.8664E-13	.8520E-13
-.2	.8385E-03	.8323E-02	.8381E-03	.1000E-01	.9066E-13	.8916E-13
-.1	.8387E-03	.8323E-02	.8382E-03	.1000E-01	.9529E-13	.9377E-13
.0	.8388E-03	.8323E-02	.8383E-03	.1000E-01	.9013E-13	.8858E-13
.1	.8388E-03	.8323E-02	.8384E-03	.1000E-01	.8803E-13	.8644E-13
.2	.8389E-03	.8323E-02	.8384E-03	.1000E-01	.9601E-13	.9437E-13
.3	.8389E-03	.8323E-02	.8385E-03	.1000E-01	.7816E-13	.7658E-13
.4	.8389E-03	.8323E-02	.8385E-03	.1000E-01	.8363E-13	.8196E-13
.5	.8390E-03	.8323E-02	.8385E-03	.1000E-01	.9096E-13	.8935E-13
.6	.8389E-03	.8323E-02	.8385E-03	.1000E-01	.1108E-12	.1093E-12
.7	.8389E-03	.8323E-02	.8385E-03	.1000E-01	.1309E-12	.1292E-12
.8	.8389E-03	.8323E-02	.8385E-03	.1000E-01	.6498E-13	.6334E-13
.9	.8389E-03	.8323E-02	.8384E-03	.1000E-01	.7668E-13	.7494E-13
1.0	.8388E-03	.8323E-02	.8384E-03	.1000E-01	.7596E-13	.7455E-13
1.1	.8388E-03	.8323E-02	.8384E-03	.1000E-01	.6712E-13	.6561E-13
1.2	.8388E-03	.8323E-02	.8384E-03	.1000E-01	.1469E-12	.1453E-12
1.3	.8387E-03	.8323E-02	.8383E-03	.1000E-01	.1283E-12	.1269E-12
1.4	.8387E-03	.8323E-02	.8383E-03	.1000E-01	.9255E-13	.9104E-13
1.5	.8386E-03	.8323E-02	.8382E-03	.1000E-01	.1193E-12	.1177E-12
1.6	.8386E-03	.8323E-02	.8382E-03	.1000E-01	.2372E-12	.2354E-12
1.7	.8385E-03	.8323E-02	.8381E-03	.1000E-01	.7615E-13	.7438E-13
1.8	.8384E-03	.8323E-02	.8381E-03	.1000E-01	.6879E-13	.6661E-13
1.9	.8384E-03	.8324E-02	.8380E-03	.1000E-01	.3280E-12	.3264E-12

Table for optimal β 's, their row-sum, and the square norm of the local truncation error functional for Cowell's 3-points usual and the corresponding β-optimal methods in $H^{(s)}_{a,b}$ space, at nodal points with a=-2, b=2, n=40, h=.1, α_0=-1, α_1=2, α_2=-1, β_0=.0833333, β_1=.833333, β_2=.0833333.

Table - 2(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.325777E-02
2	.961538E-02	.710710E-02
3	.769231E-02	.538832E-02
4	.448718E-02	.254809E-02
5	.108974E-01	.601694E-02
6	.466667E-02	.307797E-02
7	.102985E-01	.937909E-02
8	.749346E-02	.635989E-02
9	.539873E-02	.401227E-02
10	.270475E-02	.857182E-03

Table for average discretisation error using Cowell's 3-points usual and the corresponding β-optimal methods in $H^{(4)}_{a,b}$-space, for 10 BVP-s with a=-2, b=2, n=40, h=.1.

Table - 3(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.475926E-02
2	.961538E-02	.954940E-02
3	.769231E-02	.763332E-02
4	.448718E-02	.443331E-02
5	.108974E-01	.107347E-01
6	.466667E-02	.461616E-02
7	.102985E-01	.102668E-01
8	.749346E-02	.745476E-02
9	.539873E-02	.535184E-02
10	.270475E-02	.263734E-02

Table for average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimalmethod in $H^{(5)}_{a,b}$-space, for 10 BVP-s with a=-2, b=2, n=40, h=.1.

The results for α-optimal method on the same equations 1-10 are not so promising.

In $H^{(m)}_{a,b}$ space, to determine the optimal coefficients $\hat{\beta}_{i,n}$, $i = \delta_{to}(1)k$ of β-optimal multistep method (20) subject to the condition

$$(22) \qquad \sum_{j=\delta_{t0}}^{k} \hat{\beta}_{j,n} = 1,$$

where α_j's are prefixed according to some consistent and stable known usual method (21) with highest degree polynomial precision, with reference to equation (15) of Chapter 1, we have to solve the system of normal equations given by

$$\hat{C}\,\hat{b} = \hat{d},$$

where

$$\hat{b} = h^2\left(\hat{\beta}_{\delta_{t0},n}, \ldots\ldots\ldots, \hat{\beta}_{k-1,n}\right)^T,$$

$$\hat{C}_{ij} = D2''(x_{n+k-j}, x_{n+k-i}) - D2''(x_{n+k-j}, x_n) - D2''(x_n, x_{n+k-i}) + D2''(x_n, x_n),$$

$$\text{for } i,j = \delta_{t0}(1)k-1,$$

$$\hat{d}_i = \sum_{j=0}^{k} \alpha_j [D2(x_{n+k-j}, x_{n+k-i}) - D2(x_{n+k-j}, x_n)] -$$

$$-h^2[D2''(x_n, x_{n+k-i}) - D2''(x_n, x_n)], \quad \text{for } i = \delta_{t0}(1)k-1,$$

and $D2(y,x)$ and $D2''(y,x)$ are given by (18) and (19). This system of equations can be solved for $h^2\hat{\beta}_{j,n}$, $j = \delta_{t0}(1)k-1$.

The following theorem characterizes the β-optimal multistep method (20) in $H^{(m)}_{a,b}$ space subject to the condition (22).

<u>Theorem 3:</u> The optimal multistep method (20) in which α_j's are prefixed and β_j's are optimized in $H^{(m)}_{a,b}$ space, subject to the condition (22) is characterized by that it is locally interpolatory for functions $\{D2(x, x_{n+k-i}) - D2(x, x_n),\ i=\delta_{t0}(1)k-1\}$, where $D2(y,x)$ is given by (18).

<u>Proof:</u> The proof follows from Theorem 3 of Chapter 1.

In the following tables we are presenting the numerical

results for β-optimal method with restriction corresponding to Cowell's usual method with function evaluation at three points. The behavior of the performance of β-optimal method with restriction, on the above 10 BVP, over Cowell's usual method is similar to that in the case of β-optimal method, discussed in section 6.3.

In $H^{(3)}_{a,b}$-space, the optimal beta coefficients and the square norm of local truncation error functional for usual and β-optimal methods with restriction are independent of points and these quantities are numerically almost the same as in the case of β-optimal method in $H^{(3)}_{a,b}$-space, discussed in section 6.3. We therefore omit the corresponding table. The following table shows the performance of usual and β-optimal methods with restriction on the above 10 BVP's.

Table - 4(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.401411E-14
2	.961538E-02	.115378E-13
3	.769231E-02	.219995E-13
4	.448718E-02	.505806E-13
5	.108974E-01	.135070E-13
6	.466667E-02	.685492E-14
7	.102985E-01	.841119E-02
8	.749346E-02	.507054E-02
9	.539873E-02	.232991E-02
10	.270475E-02	.207524E-02

Table for average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal method with restriction, in $H^{(3)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

We are presenting the numerical results, in Tables 5 and 5(i) for $H^{(4)}_{a,b}$ space and in Tables 6 and 6(i) for $H^{(5)}_{a,b}$ space for the same 10 BVP's.

Table - 5

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\lVert T_n \rVert^2$	$\lVert \hat{T}_n \rVert^2$
-1.9	.1010E-02	.7988E-02	.1002E-02	.1000E-01	.1455E-09	.1263E-09
-1.8	.1009E-02	.7989E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.7	.1008E-02	.7990E-02	.1002E-02	.1000E-01	.1455E-09	.1264E-09
-1.6	.1008E-02	.7991E-02	.1002E-02	.1000E-01	.1455E-09	.1265E-09
-1.5	.1007E-02	.7991E-02	.1001E-02	.1000E-01	.1455E-09	.1265E-09
-1.4	.1007E-02	.7992E-02	.1001E-02	.1000E-01	.1455E-09	.1265E-09
-1.3	.1006E-02	.7992E-02	.1001E-02	.1000E-01	.1455E-09	.1266E-09
-1.2	.1006E-02	.7993E-02	.1001E-02	.1000E-01	.1455E-09	.1266E-09
-1.1	.1006E-02	.7993E-02	.1001E-02	.1000E-01	.1455E-09	.1266E-09
-1.0	.1005E-02	.7994E-02	.1001E-02	.1000E-01	.1455E-09	.1266E-09
-.9	.1005E-02	.7994E-02	.1001E-02	.1000E-01	.1455E-09	.1266E-09
-.8	.1005E-02	.7994E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.7	.1005E-02	.7994E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.6	.1004E-02	.7995E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.5	.1004E-02	.7995E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.4	.1004E-02	.7995E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.3	.1004E-02	.7995E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.2	.1004E-02	.7995E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
-.1	.1004E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
.0	.1004E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
.1	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
.2	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
.3	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1267E-09
.4	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
.5	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
.6	.1003E-02	.7996E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
.7	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
.8	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
.9	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
1.0	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1455E-09	.1268E-09
1.1	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1454E-09	.1267E-09
1.2	.1003E-02	.7997E-02	.1001E-02	.1000E-01	.1454E-09	.1267E-09
1.3	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1455E-09	.1268E-09
1.4	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1455E-09	.1269E-09
1.5	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1456E-09	.1269E-09
1.6	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1456E-09	.1269E-09
1.7	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1457E-09	.1270E-09
1.8	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1457E-09	.1270E-09
1.9	.1002E-02	.7997E-02	.1000E-02	.1000E-01	.1458E-09	.1272E-09

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using Cowell's 3-points usual and the corresponding β-optimal method methods with restriction, in $H^{(4)}_{a,b}$-space, at the nodal points, with a=-2, b=2, n=40, h=.1, α_0=-1, α_1=2, α_2=-1, β_0=.833333, β_1=.833333, β_2=.833333.

Table - 6

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.9	.8363E-03	.8327E-02	.8363E-03	.1000E-01	.8830E-13	.8736E-13
-1.8	.8361E-03	.8328E-02	.8361E-03	.1000E-01	.8795E-13	.8708E-13
-1.7	.8360E-03	.8328E-02	.8360E-03	.1000E-01	.8759E-13	.8676E-13
-1.6	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.8816E-13	.8735E-13
-1.5	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.8860E-13	.8779E-13
-1.4	.8361E-03	.8328E-02	.8359E-03	.1000E-01	.8861E-13	.8779E-13
-1.3	.8361E-03	.8328E-02	.8360E-03	.1000E-01	.8776E-13	.8693E-13
-1.2	.8362E-03	.8328E-02	.8361E-03	.1000E-01	.8804E-13	.8718E-13
-1.1	.8363E-03	.8328E-02	.8362E-03	.1000E-01	.8808E-13	.8720E-13
-1.0	.8364E-03	.8327E-02	.8362E-03	.1000E-01	.8705E-13	.8613E-13
-.9	.8365E-03	.8327E-02	.8363E-03	.1000E-01	.8773E-13	.8679E-13
-.8	.8366E-03	.8327E-02	.8364E-03	.1000E-01	.9176E-13	.9078E-13
-.7	.8367E-03	.8327E-02	.8365E-03	.1000E-01	.9188E-13	.9089E-13
-.6	.8368E-03	.8327E-02	.8366E-03	.1000E-01	.8998E-13	.8896E-13
-.5	.8368E-03	.8327E-02	.8366E-03	.1000E-01	.9181E-13	.9078E-13
-.4	.8369E-03	.8326E-02	.8367E-03	.1000E-01	.8925E-13	.8820E-13
-.3	.8369E-03	.8326E-02	.8367E-03	.1000E-01	.8664E-13	.8557E-13
-.2	.8369E-03	.8326E-02	.8367E-03	.1000E-01	.9066E-13	.8960E-13
-.1	.8369E-03	.8326E-02	.8367E-03	.1000E-01	.9529E-13	.9424E-13
.0	.8369E-03	.8326E-02	.8367E-03	.1000E-01	.9013E-13	.8910E-13
.1	.8368E-03	.8326E-02	.8367E-03	.1000E-01	.8803E-13	.8697E-13
.2	.8368E-03	.8327E-02	.8367E-03	.1000E-01	.9601E-13	.9496E-13
.3	.8368E-03	.8327E-02	.8366E-03	.1000E-01	.7816E-13	.7714E-13
.4	.8367E-03	.8327E-02	.8366E-03	.1000E-01	.8363E-13	.8258E-13
.5	.8367E-03	.8327E-02	.8365E-03	.1000E-01	.9096E-13	.8993E-13
.6	.8366E-03	.8327E-02	.8365E-03	.1000E-01	.1108E-12	.1099E-12
.7	.8366E-03	.8327E-02	.8365E-03	.1000E-01	.1309E-12	.1298E-12
.8	.8365E-03	.8327E-02	.8364E-03	.1000E-01	.6498E-13	.6401E-13
.9	.8365E-03	.8327E-02	.8364E-03	.1000E-01	.7668E-13	.7575E-13
1.0	.8364E-03	.8327E-02	.8363E-03	.1000E-01	.7596E-13	.7524E-13
1.1	.8364E-03	.8327E-02	.8363E-03	.1000E-01	.6712E-13	.6632E-13
1.2	.8363E-03	.8327E-02	.8362E-03	.1000E-01	.1469E-12	.1463E-12
1.3	.8363E-03	.8328E-02	.8362E-03	.1000E-01	.1283E-12	.1272E-12
1.4	.8362E-03	.8328E-02	.8361E-03	.1000E-01	.9255E-13	.9159E-13
1.5	.8362E-03	.8328E-02	.8361E-03	.1000E-01	.1193E-12	.1183E-12
1.6	.8361E-03	.8328E-02	.8360E-03	.1000E-01	.2372E-12	.2358E-12
1.7	.8361E-03	.8328E-02	.8360E-03	.1000E-01	.7615E-13	.7538E-13
1.8	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.6879E-13	.6732E-13
1.9	.8360E-03	.8328E-02	.8359E-03	.1000E-01	.3280E-12	.3273E-12

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using Cowell's 3-points usual and the corresponding β-optimal methods with restriction, in $H^{(5)}_{a,b}$-space, at the nodal points, with a=-2, b=2, n=40, h=.1, α_0=-1, α_1=2, α_2=-1, β_0=.833333, β_1=.833333, β_2=.833333.

Table - 5(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.368457E-02
2	.961538E-02	.753787E-02
3	.769231E-02	.604319E-02
4	.448718E-02	.354015E-02
5	.108974E-01	.808629E-02
6	.466667E-02	.355873E-02
7	.102985E-01	.981491E-02
8	.749346E-02	.687194E-02
9	.539873E-02	.461103E-02
10	.270475E-02	.147793E-02

Table for average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal method with restriction, in $H^{(4)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

Table - 6(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.478223E-02
2	.961538E-02	.957449E-02
3	.769231E-02	.766364E-02
4	.448718E-02	.447275E-02
5	.108974E-01	.108284E-01
6	.466667E-02	.464119E-02
7	.102985E-01	.102867E-01
8	.749346E-02	.747828E-02
9	.539873E-02	.537951E-02
10	.270475E-02	.267498E-02

Table for average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods with restriction, in $H^{(5)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

6.4 Optimal Multistep Methods in $H^{(m)}_{a,b}$-Space Interpolatory for Polynomials.

In section 4.4, we have given an approach for determining the optimal multistep methods interpolatory for polynomials of certain degree, in $H^2(C_r)$ space. In $H^{(m)}_{a,b}$ space, the equispaced nodal points x_{n+k-i}, $i=0(1)k$ are along a straight line in an interval [a,b]. To find the β-optimal methods interpolatory for polynomials of certain degree we have to solve the system of equations, $\hat{C}\,\hat{b} = \hat{d}$,

where $\hat{b} = \left(\hat{\gamma}_{q-1,n}, \hat{\gamma}_{q,n}, \ldots\ldots, \hat{\gamma}_{k-\delta_{t0},n}\right)^T$,

$$\hat{c}_{ij} = h^2 \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\, {}^{i}C_l\, {}^{j}C_m\, D2''(x_{n+k-\delta_{t0}-m}, \bar{x}_{n+k-\delta_{t0}-l}),$$

$$\hat{d}_i = -h^2 \sum_{j=0}^{q-2} \gamma_j^u \sum_{m=0}^{j} \sum_{l=0}^{i} (-1)^{l+m}\, {}^{i}C_l\, {}^{j}C_m\, D2''(x_{n+k-\delta_{t0}-m}, \bar{x}_{n+k-\delta_{t0}-l})$$

$$- \sum_{j=0}^{k} \alpha_j \sum_{l=0}^{i} (-1)^{l}\, {}^{i}C_l\, D2(x_{n+k-j}, \bar{x}_{n+k-\delta_{t0}-l}), \quad i,j=q-1(1)k-\delta_{t0},$$

where γ_j^u, $j=0(1)q-2$ are equal to β_j, $j=0(1)q-2$ in the usual method and $D2(y,x)$ and $D2''(y,x)$ are given by (18) and (19).

In $H_{a,b}^{(3)}$-space, the numerical values of optimal beta coefficients and the square norm of local truncation error functionals for usual and β-optimal methods interpolatory for polynomials of degree 3 are independent of points and numerically these quantities are nearly the same as in the case of β-optimal method in $H_{a,b}^{(3)}$-space, presented in section 6.3. The corresponding table, therefore is omitted.

Table - 7(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.244860E-13
2	.961538E-02	.470848E-13
3	.769231E-02	.169158E-12
4	.448718E-02	.274652E-13
5	.108974E-01	.115902E-12
6	.466667E-02	.101750E-12
7	.236952E-01	.222815E-01
8	.102985E-01	.841119E-02
9	.749346E-02	.507054E-02
10	.539873E-02	.232991E-02
11	.270475E-02	.207524E-02
12	.187310E-02	.402683E-02
13	.127316E-02	.596774E-02

Table for average discretisation errors using Cowell's 3-points usual and β-optimal method interpolatory for polynomials of degree 3, in $H_{a,b}^{(3)}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

Table - 8

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.9	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.8	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.7	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.6	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.5	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.4	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.3	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.2	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.1	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-1.0	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.9	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.8	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.7	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.6	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.5	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.4	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.3	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.2	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
-.1	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.0	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.1	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.2	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.3	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1269E-09
.4	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.5	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.6	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.7	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.8	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
.9	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
1.0	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
1.1	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1454E-09	.1269E-09
1.2	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1454E-09	.1269E-09
1.3	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1269E-09
1.4	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1455E-09	.1270E-09
1.5	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1456E-09	.1270E-09
1.6	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1456E-09	.1271E-09
1.7	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1457E-09	.1271E-09
1.8	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1457E-09	.1272E-09
1.9	.1000E-02	.8000E-02	.1000E-02	.1000E-01	.1458E-09	.1273E-09

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using Cowell's 3-points usual and the corresponding β-optimal methods interpolatory for polynomials of degree 3, in $H^{(4)}_{a,b}$-space, at the nodal points, with a=-2, b=2, n=40, h=.1, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=.833333$, $\beta_1=.833333$, $\beta_2=.833333$, $\gamma_1=1$, $\gamma_2=-1$, $\gamma_3=1/12$.

Table - 9

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.9	.8363E-03	.8327E-02	.8363E-03	.1000E-01	.8830E-13	.8736E-13
-1.8	.8360E-03	.8328E-02	.8360E-03	.1000E-01	.8795E-13	.8710E-13
-1.7	.8358E-03	.8328E-02	.8358E-03	.1000E-01	.8759E-13	.8681E-13
-1.6	.8356E-03	.8329E-02	.8356E-03	.1000E-01	.8816E-13	.8743E-13
-1.5	.8355E-03	.8329E-02	.8355E-03	.1000E-01	.8860E-13	.8792E-13
-1.4	.8353E-03	.8329E-02	.8353E-03	.1000E-01	.8861E-13	.8797E-13
-1.3	.8352E-03	.8330E-02	.8352E-03	.1000E-01	.8776E-13	.8716E-13
-1.2	.8351E-03	.8330E-02	.8351E-03	.1000E-01	.8804E-13	.8747E-13
-1.1	.8350E-03	.8330E-02	.8350E-03	.1000E-01	.8808E-13	.8754E-13
-1.0	.8349E-03	.8330E-02	.8349E-03	.1000E-01	.8705E-13	.8654E-13
-.9	.8349E-03	.8330E-02	.8349E-03	.1000E-01	.8773E-13	.8725E-13
-.8	.8348E-03	.8330E-02	.8348E-03	.1000E-01	.9176E-13	.9129E-13
-.7	.8347E-03	.8331E-02	.8347E-03	.1000E-01	.9188E-13	.9144E-13
-.6	.8347E-03	.8331E-02	.8347E-03	.1000E-01	.8998E-13	.8956E-13
-.5	.8346E-03	.8331E-02	.8346E-03	.1000E-01	.9181E-13	.9140E-13
-.4	.8346E-03	.8331E-02	.8346E-03	.1000E-01	.8925E-13	.8884E-13
-.3	.8345E-03	.8331E-02	.8345E-03	.1000E-01	.8664E-13	.8627E-13
-.2	.8345E-03	.8331E-02	.8345E-03	.1000E-01	.9066E-13	.9031E-13
-.1	.8344E-03	.8331E-02	.8344E-03	.1000E-01	.9529E-13	.9494E-13
.0	.8344E-03	.8331E-02	.8344E-03	.1000E-01	.9013E-13	.8980E-13
.1	.8344E-03	.8331E-02	.8344E-03	.1000E-01	.8803E-13	.8767E-13
.2	.8343E-03	.8331E-02	.8343E-03	.1000E-01	.9601E-13	.9568E-13
.3	.8343E-03	.8331E-02	.8343E-03	.1000E-01	.7816E-13	.7789E-13
.4	.8343E-03	.8331E-02	.8343E-03	.1000E-01	.8363E-13	.8331E-13
.5	.8342E-03	.8332E-02	.8342E-03	.1000E-01	.9096E-13	.9064E-13
.6	.8342E-03	.8332E-02	.8342E-03	.1000E-01	.1108E-12	.1106E-12
.7	.8342E-03	.8332E-02	.8342E-03	.1000E-01	.1309E-12	.1305E-12
.8	.8342E-03	.8332E-02	.8342E-03	.1000E-01	.6498E-13	.6464E-13
.9	.8342E-03	.8332E-02	.8342E-03	.1000E-01	.7668E-13	.7641E-13
1.0	.8341E-03	.8332E-02	.8341E-03	.1000E-01	.7596E-13	.7577E-13
1.1	.8341E-03	.8332E-02	.8341E-03	.1000E-01	.6712E-13	.6714E-13
1.2	.8341E-03	.8332E-02	.8341E-03	.1000E-01	.1469E-12	.1468E-12
1.3	.8341E-03	.8332E-02	.8341E-03	.1000E-01	.1283E-12	.1281E-12
1.4	.8341E-03	.8332E-02	.8341E-03	.1000E-01	.9255E-13	.9247E-13
1.5	.8340E-03	.8332E-02	.8340E-03	.1000E-01	.1193E-12	.1190E-12
1.6	.8340E-03	.8332E-02	.8340E-03	.1000E-01	.2372E-12	.2365E-12
1.7	.8340E-03	.8332E-02	.8340E-03	.1000E-01	.7615E-13	.7555E-13
1.8	.8340E-03	.8332E-02	.8340E-03	.1000E-01	.6879E-13	.6822E-13
1.9	.8340E-03	.8332E-02	.8340E-03	.1000E-01	.3280E-12	.3276E-12

Table for optimal β's, their row-sum and the square norm of local truncation error functionals using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, in $H^{(5)}_{a,b}$-space, at the nodal points, with a=-2, b=2, n=40, h=.1, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_0=.833333$, $\beta_1=.833333$, $\beta_2=.833333$, $\gamma_0=1$, $\gamma_1=-1$, $\gamma_2=1/12$.

Table - 8(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.384615E-02
2	.961538E-02	.769231E-02
3	.769231E-02	.615385E-02
4	.448718E-02	.358974E-02
5	.108974E-01	.871795E-02
6	.466667E-02	.373333E-02
7	.102985E-01	.992101E-02
8	.749346E-02	.700888E-02
9	.539873E-02	.478497E-02
10	.270475E-02	.174875E-02

Table for average discretisation errors using Cowell's 3-points usual and the corresponding β-optimal methods interpolatory for polynomials of degree 3, in $H^{(4)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

Table - 9(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.480769E-02	.480242E-02
2	.961538E-02	.960272E-02
3	.769231E-02	.768121E-02
4	.448718E-02	.447948E-02
5	.108974E-01	.108866E-01
6	.466667E-02	.466170E-02
7	.102985E-01	.102970E-01
8	.749346E-02	.749139E-02
9	.539873E-02	.539595E-02
10	.270475E-02	.269993E-02

Table for average discretisation errors using Cowell's 3-points usual method and the corresponding β-optimal method interpolatory for polynomials of degree 3, in $H^{(5)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

6.5 Optimal Multistep Methods in $H^{(m)}_{a,b}$-Space Interpolatory for a Set of Preassigned Functions.

To obtain the coefficients $\hat{\beta}^F_{j,n}$, $j = \delta_{t0}(1)k$ of a β-optimal multistep method

$$(23) \qquad \sum_{j=0}^{k} \alpha_j \, y_{n+k-j} + h^2 \sum_{j=\delta_{t0}}^{k} \hat{\beta}^F_{j,n} \, f_{n+k-j} = 0$$

corresponding to the usual method (21) of highest degree polynomial precision, in $H^{(m)}_{a,b}$ space with prefixed α_j's, interpolatory for q number of linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$ we have to solve a system of linear equations given in the matrix form

$$\begin{bmatrix} A & F^* \\ F & 0 \end{bmatrix} \begin{bmatrix} b \\ \lambda \end{bmatrix} = \begin{bmatrix} c \\ f \end{bmatrix},$$

where $A = (A_{ij})$, with $A_{ij} = D2''(x_{n+k-j}, x_{n+k-i})$, $i,j=\delta_{t0}(1)k$,

$F = (F_{ij})$, with $F_{ij} = f_i''\ (x_{n+k-j})$, $i=1(1)q$, $j=\delta_{t0}(1)k$,

$b = h^2\left(\hat{\beta}^F_{\delta_{t0},n}, \hat{\beta}^F_{\delta_{t0}+1,n}, \ldots, \hat{\beta}^F_{k,n}\right)^T$,

$\lambda = (\ \lambda_1, \lambda_2, \ldots, \lambda_q\ )^T$,

$c = (c_{\delta_{t0}}, \ldots, c_k)^T$; with $c_i = -\sum_{j=0}^{k} \alpha_j D2(x_{n+k-j}, x_{n+k-i})$, $i=\delta_{t0}(1)k$,

and

$f = (\tilde{f}_1, \tilde{f}_2, \ldots, \tilde{f}_q)^T$; with $\tilde{f}_i = -\sum_{j=0}^{k} \alpha_j f_i(x_{n+k-j})$.

This method is characterized as follows.

<u>Theorem 9:</u> The β-optimal multistep method (16), in $H^{(m)}_{a,b}$ space, interpolatory for linearly independent arbitrary functions $f_1, f_2, \ldots, f_q$ is characterized by that it is locally interpolatory for the functions

$$\{\ f_1, f_2, \ldots, f_q\ \} \cup \{\ h_i,\ i = \delta_{t0}(1)k-q\ \},$$

where $h_i(x) = D2(x, x_{n+k-i}) - \sum_{j=k-q+1}^{k} \bar{g}_{j+q-k,\, i+1-\delta_{t0}} D2(x, x_{n+k-j})$,

and

$$G = P^{-1}E = (g_{ij})_{\substack{i=1(1)q \\ j=1(1)k-q-\delta_{t0}+1}},$$

$$P = \left(f_i''\ (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=k-q+1(1)k}}, \quad E = \left(f_i''\ (x_{n+k-j})\right)_{\substack{i=1(1)q \\ j=\delta_{t0}(1)k-q}},$$

where $D2(x, x_{n+k-i})$, $i = \delta_{t0}(1)k-q$ are given by (18).

Proof: The proof follows from Theorem 8 of Chapter 1.

The following tables are for average discretisation errors for the usual method with highest degree polynomial precision and the beta optimal method interpolatory for linearly independent functions, exp(3.6x) and exp(-3.6x) on 6 BVP-s with differential equations of the form $\frac{d^2y}{dx^2} = f(x,y) = g(x)$, having the true solutions given as follows.

1. exp(3.6x)
2. exp(-3.6x)
3. exp(3.59x)
4. exp(-3.59x)
5. exp(3.61x)
6. exp(-3.61x)

For this implementation, we are presenting the numerical results for some more values of h.

Table-10(i)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.411111E-01	.298928E-11
2	.411111E-01	.563743E-13
3	.424271E-01	.313737E-01
4	.424271E-01	.261371E-01
5	.398346E-01	.300258E-01
6	.398346E-01	.250216E-01

In $H^{(3)}_{a,b}$-space, a=-2, b=2, h=.1

Table-10(ii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.661409E+00	.118234E-11
2	.661409E+00	.443688E-13
3	.682516E+00	.797048E-01
4	.682516E+00	.455930E-01
5	.640932E+00	.762205E-01
6	.640932E+00	.436243E-01

In $H^{(3)}_{a,b}$-space, a=-2, b=2, h=.2

Table-10(iii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.103140E+02	.398868E-13
2	.103140E+02	.812012E-13
3	.106393E+02	.168280E+00
4	.106393E+02	.102169E+00
5	.999829E+01	.160507E+00
6	.999829E+01	.973143E-01

In $H^{(3)}_{a,b}$-space, a=-2, b=2, h=.4

Table-10(iv)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.244472E+02	.825927E-14
2	.244472E+02	.881116E-13
3	.252119E+02	.250026E+00
4	.252119E+02	.175963E+00
5	.237048E+02	.238187E+00
6	.237048E+02	.167366E+00

In $H^{(3)}_{a,b}$-space, a=-2, b=2, h=.5

Table-11(i)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.411111E-01	.296837E-11
2	.411111E-01	.541711E-13
3	.424271E-01	.463545E-03
4	.424271E-01	.245588E-03
5	.398346E-01	.440861E-03
6	.398346E-01	.232666E-03

In $H^{(4)}_{a,b}$-space, a=-2, b=2, h=.1

Table-11(ii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.661409E+00	.133426E-11
2	.661409E+00	.313977E-13
3	.682516E+00	.427492E-02
4	.682516E+00	.372993E-02
5	.640932E+00	.405298E-02
6	.640932E+00	.353237E-02

In $H^{(4)}_{a,b}$-space, a=-2, b=2, h=.2

Table-11(iii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.103140E+02	.225625E-13
2	.103140E+02	.858510E-13
3	.106393E+02	.560321E-01
4	.106393E+02	.544066E-01
5	.999829E+01	.531115E-01
6	.999829E+01	.515581E-01

In $H^{(4)}_{a,b}$-space, a=-2, b=2, h=.4

Table-11(iv)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.244472E+02	.799559E-14
2	.244472E+02	.245784E-13
3	.252119E+02	.125536E+00
4	.252119E+02	.123319E+00
5	.237048E+02	.119040E+00
6	.237048E+02	.116921E+00

In $H^{(4)}_{a,b}$-space, a=-2, b=2, h=.5

Table-12(i)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.411111E-01	.300638E-11
2	.411111E-01	.540470E-13
3	.424271E-01	.602654E-03
4	.424271E-01	.230377E-03
5	.398346E-01	.220966E-03
6	.398346E-01	.218073E-03

In $H^{(5)}_{2,c}$-space, a=-2, b=2, h=.1

Table-12(ii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.661409E+00	.118219E-11
2	.661409E+00	.478986E-13
3	.682516E+00	.615306E-03
4	.682516E+00	.364846E-02
5	.640932E+00	.349374E-02
6	.640932E+00	.345426E-02

In $H^{(5)}_{2,c}$-space, a=-2, b=2, h=.2

Table-12(iii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.103140E+02	.290111E-13
2	.103140E+02	.123470E-12
3	.106393E+02	.636403E-03
4	.106393E+02	.534976E-01
5	.999829E+01	.511338E-01
6	.999829E+01	.506869E-01

In $H^{(5)}_{2,c}$-space, a=-2, b=2, h=.4

Table-12(iv)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.244472E+02	.624203E-13
2	.244472E+02	.478742E-13
3	.252119E+02	.644939E-03
4	.252119E+02	.121250E+00
5	.237048E+02	.115745E+00
6	.237048E+02	.114938E+00

In $H^{(5)}_{2,c}$-space, a=-2, b=2, h=.5

Table-13(i)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.411111E-01	.299115E-11
2	.411111E-01	.596382E-13
3	.424271E-01	.232631E-03
4	.424271E-01	.226527E-03
5	.398346E-01	.220219E-03
6	.398346E-01	.214386E-03

In $H^{(6)}_{a,b}$-space, a=-2, b=2, h=.1

Table-13(ii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.661409E+00	.130226E-11
2	.661409E+00	.422933E-13
3	.682516E+00	.368304E-02
4	.682516E+00	.358649E-02
5	.640932E+00	.348718E-02
6	.640932E+00	.339492E-02

In $H^{(6)}_{a,b}$-space, a=-2, b=2, h=.2

Table-13(iii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.103140E+02	.288784E-13
2	.103140E+02	.213345E-13
3	.106393E+02	.539174E-01
4	.106393E+02	.525345E-01
5	.999829E+01	.510863E-01
6	.999829E+01	.497645E-01

In $H^{(6)}_{a,b}$-space, a=-2, b=2, h=.4

Table-13(iv)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.244472E+02	.252645E-12
2	.244472E+02	.183812E-12
3	.252119E+02	.122021E+00
4	.252119E+02	.118993E+00
5	.237048E+02	.115671E+00
6	.237048E+02	.112775E+00

In $H^{(6)}_{a,b}$-space, a=-2, b=2, h=.5

However, the square norm of local truncation error functionals for β-optimal method interpolatory for exp(±3.6x) in $H^{(4)}_{a,b}$, $H^{(5)}_{a,b}$ and $H^{(6)}_{a,b}$ spaces are not being less than those for the corresponding usual method with highest degree polynomial precision. Truly

speaking, these two kinds of usual and optimal methods are not comparable. These two methods will be comparable if we choose usual method as a method with function evaluation at three points which is interpolatory for x^2 and the two other functions for which the optimal method is made interpolatory.

In the following tables we are presenting the numerical results for the usual method with function evaluation at three points which is interpolatory for x^2, cos(12x), sin(12x) and the corresponding β-optimal method interpolatory for cos(12x), sin(12x) on 6 BVP-s with differential equations of the form $\frac{d^2y}{dx^2} = f(x,y)$, having the true solutions given as follows.

1. sin12x
2. cos12x
3. sin11.9x
4. cos11.9x
5. sin11.8x
6. cos11.8x

Although in $H_{a,b}^{(3)}$-space, the square norm of local truncation error functional for the usual method is close to that for the optimal method, the absolute average discretisation error for the optimal method is less than that for the usual method. But in $H_{a,b}^{(m)}$-space, $m\geq4$, the square norm of local truncation error functionals for usual and optimal methods are numerically nearly the same, and the absolute average discretisation error for these two methods are almost same including some round-off errors. We therefore omit the corresponding tables.

Table - 14

x_n	β_{0n}	β_{1n}	β_{2n}	r-sum
-1.9	.896943E-01	.820611E+00	.896943E-01	.100410E-01
-1.8	.896943E-01	.820611E+00	.896943E-01	.100375E-01
-1.7	.896943E-01	.820611E+00	.896943E-01	.100345E-01
-1.6	.896943E-01	.820611E+00	.896943E-01	.100320E-01
-1.5	.896943E-01	.820611E+00	.896943E-01	.100298E-01
-1.4	.896943E-01	.820611E+00	.896943E-01	.100279E-01
-1.3	.896943E-01	.820611E+00	.896943E-01	.100263E-01
-1.2	.896943E-01	.820611E+00	.896943E-01	.100248E-01
-1.1	.896943E-01	.820611E+00	.896943E-01	.100234E-01
-1.0	.896943E-01	.820611E+00	.896943E-01	.100222E-01
-.9	.896943E-01	.820611E+00	.896943E-01	.100212E-01
-.8	.896943E-01	.820611E+00	.896943E-01	.100202E-01
-.7	.896943E-01	.820611E+00	.896943E-01	.100193E-01
-.6	.896943E-01	.820611E+00	.896943E-01	.100185E-01
-.5	.896943E-01	.820611E+00	.896943E-01	.100177E-01
-.4	.896943E-01	.820611E+00	.896943E-01	.100170E-01
-.3	.896943E-01	.820611E+00	.896943E-01	.100164E-01
-.2	.896943E-01	.820611E+00	.896943E-01	.100158E-01
-.1	.896943E-01	.820611E+00	.896943E-01	.100153E-01
.0	.896943E-01	.820611E+00	.896943E-01	.100147E-01
.1	.896943E-01	.820611E+00	.896943E-01	.100143E-01
.2	.896943E-01	.820611E+00	.896943E-01	.100138E-01
.3	.896943E-01	.820611E+00	.896943E-01	.100134E-01
.4	.896943E-01	.820611E+00	.896943E-01	.100130E-01
.5	.896943E-01	.820611E+00	.896943E-01	.100126E-01
.6	.896943E-01	.820611E+00	.896943E-01	.100123E-01
.7	.896943E-01	.820611E+00	.896943E-01	.100119E-01
.8	.896943E-01	.820611E+00	.896943E-01	.100116E-01
.9	.896943E-01	.820611E+00	.896943E-01	.100113E-01
1.0	.896943E-01	.820611E+00	.896943E-01	.100110E-01
1.1	.896943E-01	.820611E+00	.896943E-01	.100108E-01
1.2	.896943E-01	.820611E+00	.896943E-01	.100105E-01
1.3	.896943E-01	.820611E+00	.896943E-01	.100103E-01
1.4	.896943E-01	.820611E+00	.896943E-01	.100100E-01
1.5	.896943E-01	.820611E+00	.896943E-01	.100098E-01
1.6	.896943E-01	.820611E+00	.896943E-01	.100096E-01
1.7	.896943E-01	.820611E+00	.896943E-01	.100094E-01
1.8	.896943E-01	.820611E+00	.896943E-01	.100092E-01
1.9	.896943E-01	.820611E+00	.896943E-01	.100090E-01

Table for β-coefficients for the usual method with function evaluation at three points, interpolatory for x^2, cos(12x), sin(12x) and their row-sum at the nodal points with a=-2, b=2, n=40, h=.1, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$.

Table - 15

x_n	$h^2\hat{\beta}_{0n}$	$h^2\hat{\beta}_{1n}$	$h^2\hat{\beta}_{2n}$	r-sum	$\|T_n\|^2$	$\|\hat{T}_n\|^2$
-1.9	.9291E-03	.8183E-02	.9291E-03	.1004E-01	.5629E-06	.5611E-06
-1.8	.9264E-03	.8185E-02	.9264E-03	.1004E-01	.5629E-06	.5613E-06
-1.7	.9240E-03	.8186E-02	.9240E-03	.1003E-01	.5629E-06	.5614E-06
-1.6	.9220E-03	.8188E-02	.9220E-03	.1003E-01	.5629E-06	.5615E-06
-1.5	.9203E-03	.8189E-02	.9203E-03	.1003E-01	.5629E-06	.5616E-06
-1.4	.9188E-03	.8190E-02	.9188E-03	.1003E-01	.5629E-06	.5617E-06
-1.3	.9175E-03	.8191E-02	.9175E-03	.1003E-01	.5629E-06	.5618E-06
-1.2	.9164E-03	.8192E-02	.9164E-03	.1002E-01	.5629E-06	.5619E-06
-1.1	.9153E-03	.8193E-02	.9153E-03	.1002E-01	.5629E-06	.5619E-06
-1.0	.9144E-03	.8193E-02	.9144E-03	.1002E-01	.5629E-06	.5620E-06
-.9	.9135E-03	.8194E-02	.9135E-03	.1002E-01	.5629E-06	.5620E-06
-.8	.9128E-03	.8195E-02	.9128E-03	.1002E-01	.5629E-06	.5621E-06
-.7	.9121E-03	.8195E-02	.9121E-03	.1002E-01	.5629E-06	.5621E-06
-.6	.9114E-03	.8196E-02	.9114E-03	.1002E-01	.5629E-06	.5621E-06
-.5	.9109E-03	.8196E-02	.9109E-03	.1002E-01	.5629E-06	.5622E-06
-.4	.9103E-03	.8196E-02	.9103E-03	.1002E-01	.5629E-06	.5622E-06
-.3	.9098E-03	.8197E-02	.9098E-03	.1002E-01	.5629E-06	.5622E-06
-.2	.9093E-03	.8197E-02	.9093E-03	.1002E-01	.5629E-06	.5622E-06
-.1	.9089E-03	.8197E-02	.9089E-03	.1002E-01	.5629E-06	.5623E-06
.0	.9085E-03	.8198E-02	.9085E-03	.1001E-01	.5629E-06	.5623E-06
.1	.9081E-03	.8198E-02	.9081E-03	.1001E-01	.5629E-06	.5623E-06
.2	.9078E-03	.8198E-02	.9078E-03	.1001E-01	.5629E-06	.5623E-06
.3	.9074E-03	.8199E-02	.9074E-03	.1001E-01	.5629E-06	.5624E-06
.4	.9071E-03	.8199E-02	.9071E-03	.1001E-01	.5629E-06	.5624E-06
.5	.9068E-03	.8199E-02	.9068E-03	.1001E-01	.5629E-06	.5624E-06
.6	.9066E-03	.8199E-02	.9066E-03	.1001E-01	.5629E-06	.5624E-06
.7	.9063E-03	.8199E-02	.9063E-03	.1001E-01	.5629E-06	.5624E-06
.8	.9061E-03	.8200E-02	.9061E-03	.1001E-01	.5629E-06	.5624E-06
.9	.9058E-03	.8200E-02	.9058E-03	.1001E-01	.5629E-06	.5624E-06
1.0	.9056E-03	.8200E-02	.9056E-03	.1001E-01	.5629E-06	.5625E-06
1.1	.9054E-03	.8200E-02	.9054E-03	.1001E-01	.5629E-06	.5625E-06
1.2	.9052E-03	.8200E-02	.9052E-03	.1001E-01	.5629E-06	.5625E-06
1.3	.9050E-03	.8200E-02	.9050E-03	.1001E-01	.5629E-06	.5625E-06
1.4	.9048E-03	.8200E-02	.9048E-03	.1001E-01	.5629E-06	.5625E-06
1.5	.9046E-03	.8201E-02	.9046E-03	.1001E-01	.5629E-06	.5625E-06
1.6	.9045E-03	.8201E-02	.9045E-03	.1001E-01	.5629E-06	.5625E-06
1.7	.9043E-03	.8201E-02	.9043E-03	.1001E-01	.5629E-06	.5625E-06
1.8	.9041E-03	.8201E-02	.9041E-03	.1001E-01	.5629E-06	.5625E-06
1.9	.9040E-03	.8201E-02	.9040E-03	.1001E-01	.5629E-06	.5625E-06

Table for optimal β's, their row-sum and the square norm of local truncation error functional for Cowell's 3-points usual and the corresponding β-optimal methods, interpolatory for cos(12x), sin(12x), in $H^{(3)}_{a,b}$ space, at the nodal points, with a=-2, b=2, n=40, h=.1, α_0=-1, α_1=2, α_2=-1, β_0=.833333, β_1=.833333, β_2=.833333.

Table-15(i)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.414802E-14	.311327E-14
2	.285788E-13	.593124E-14
3	.116894E-03	.955821E-04
4	.107057E-03	.862352E-04
5	.234438E-03	.190407E-03
6	.201188E-03	.163068E-03

In $H^{(3)}_{2,c}$-space, a=-2, b=2, h=.1

Table-15(ii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.312807E-13	.183479E-14
2	.736472E-14	.597840E-14
3	.277344E-02	.279421E-02
4	.261586E-02	.263423E-02
5	.546854E-02	.551106E-02
6	.465446E-02	.468707E-02

In $H^{(3)}_{2,c}$-space, a=-2, b=2, h=.2

Table-15(iii)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.228048E-13	.770885E-14
2	.255243E-13	.957722E-14
3	.433940E+00	.431640E+00
4	.349018E+00	.347560E+00
5	.815712E+00	.811524E+00
6	.580495E+00	.578334E+00

In $H^{(3)}_{2,c}$-space, a=-2, b=2, h=.4

Table-15(iv)

eqn	$\bar{e}_u$	$\bar{e}_o$
1	.287833E-13	.385882E-14
2	.208881E-12	.249007E-14
3	.115117E+02	.244841E+00
4	.681617E+02	.422203E+00
5	.270802E+02	.574618E+00
6	.136431E+03	.840303E+00

In $H^{(3)}_{2,c}$-space, a=-2, b=2, h=.5

Now in Table 16, we are presenting the numerical results for Stormer's usual method with function evaluation at one point and the corresponding β-optimal method on 2 BVP-s with differential equations of the form $\frac{d^2y}{dx^2} = f(x,y) = g(x)$, whose exact solutions are given by:

(1) $y(x) = \sin 4x$,

(2) $y(x) = \cos 4x$.

In $H^{(m)}_{a,b}$ space with m≥4, the numerical results suggest that there is no remarkable difference in the square norm of local truncation error functionals for the above usual method and the optimal method. So, in this case we are interested in the numerical results for $H^{(3)}_{a,b}$ space only.

Table - 16

x_n	$h^2\hat{\beta}_{1n}$	$\lVert T_n \rVert^2$	$\lVert \hat{T}_n \rVert^2$
-1.9	.9848E-02	.1000E-05	.9747E-06
-1.8	.9861E-02	.1000E-05	.9769E-06
-1.7	.9872E-02	.1000E-05	.9786E-06
-1.6	.9881E-02	.1000E-05	.9802E-06
-1.5	.9889E-02	.1000E-05	.9815E-06
-1.4	.9896E-02	.1000E-05	.9826E-06
-1.3	.9902E-02	.1000E-05	.9837E-06
-1.2	.9907E-02	.1000E-05	.9846E-06
-1.1	.9912E-02	.1000E-05	.9854E-06
-1.0	.9917E-02	.1000E-05	.9861E-06
-.9	.9921E-02	.1000E-05	.9868E-06
-.8	.9924E-02	.1000E-05	.9874E-06
-.7	.9928E-02	.1000E-05	.9879E-06
-.6	.9931E-02	.1000E-05	.9884E-06
-.5	.9933E-02	.1000E-05	.9889E-06
-.4	.9936E-02	.1000E-05	.9893E-06
-.3	.9938E-02	.1000E-05	.9897E-06
-.2	.9940E-02	.1000E-05	.9901E-06
-.1	.9943E-02	.1000E-05	.9904E-06
.0	.9944E-02	.1000E-05	.9907E-06
.1	.9946E-02	.1000E-05	.9910E-06
.2	.9948E-02	.1000E-05	.9913E-06
.3	.9949E-02	.1000E-05	.9916E-06
.4	.9951E-02	.1000E-05	.9918E-06
.5	.9952E-02	.1000E-05	.9921E-06
.6	.9954E-02	.1000E-05	.9923E-06
.7	.9955E-02	.1000E-05	.9925E-06
.8	.9956E-02	.1000E-05	.9927E-06
.9	.9957E-02	.1000E-05	.9929E-06
1.0	.9958E-02	.1000E-05	.9931E-06
1.1	.9959E-02	.1000E-05	.9932E-06
1.2	.9960E-02	.1000E-05	.9934E-06
1.3	.9961E-02	.1000E-05	.9935E-06
1.4	.9962E-02	.1000E-05	.9937E-06
1.5	.9963E-02	.1000E-05	.9938E-06
1.6	.9964E-02	.1000E-05	.9940E-06
1.7	.9965E-02	.1000E-05	.9941E-06
1.8	.9965E-02	.1000E-05	.9942E-06
1.9	.9966E-02	.1000E-05	.9943E-06

Table for optimal β and the square norm of local truncation error functional for Stormer's 1-point usual and the corresponding β-optimal methods in $H^{(3)}_{a,b}$ space, at the nodal points, with $a=-2$, $b=2$, $n=40$, $h=.1$, $\alpha_0=-1$, $\alpha_1=2$, $\alpha_2=-1$, $\beta_1=1$.

Table - 16(i)

eqn.	$\bar{e}_u$	$\bar{e}_o$
1	.985155E-02	.594575E-02
2	.910997E-02	.540173E-02

Table for average discretisation errors using Stormer's 1-point usual and the corresponding β-optimal methods in $H^{(3)}_{a,b}$-space, on 10 BVP-s with a=-2, b=2, n=40, h=.1.

REFERENCES

[1] Aguado, P.M. and Correas, J.M., A stabilization process for linear multistep methods with variable coefficients, Proceedings of second conference on differential equations and their applications I, (1979).

[2] Aguado, P.M., On the A-stability of Linear Multistep Method with variable coefficients, Differential equations and applications, Proc. 5th Congr., Tenerige/Spain 187-198, (1984).

[3] Andreassen, D., On K-step methods with almost constant coefficients, BIT, Nordisk Tidskr. Inform.-behandl., 13, 265-271, (1973).

[4] Aronszajn, N., Theory of reproducing kernels, Trans. Amer. Math. Soc., 68, 337-404, (1950).

[5] Asfar, O.R. and Hussein, A.M., Numerical solution of linear two-point boundary value problems via the fundamental matrix method, International journal for Numerical Methods in Engineering, 28, 1205-1216, (1989).

[6] Axelsson, Owe, A class of A-stable methods, BIT, Nordisk Tidskr. Inform.- Behandl., 9, 185-190, (1969).

[7] Baboo, Sabita Nath, Finite difference methods and their convergence for a class of two-point boundary value problems with periodic boundary conditions, Ph.D. Thesis, School of Computer and Systems Sciences, Jawaharlal Nehru University, New Delhi, (1992).

[8] Bakhvalov, N.S.,Numerical Methods, Mir Publishers, MOscow, (Eng. Edition), (1977).

[9] Balajan, N.M. and Molokovic, J.M., On the question of difference schemes with a higher order of precision for an ordinary differential equation with a regular singularity, Soviet Math. 7, 7-14, (1976).

[10] Barnhill, R.E., The convergence of quadratures on complex contours, SIAM J. Numer. Anal., Ser. B, 2, 321-336, (1965).

[11] Barnhill, R.E., Complex quadratures with remainders of minimum norm, Numer. Math., 7, 384-390, (1965)

[12] Barnhill, R.E., Optimal quadratures in $L^2(\epsilon_\rho)$I, SIAM J. Numer. Anal., 4, 390-397, (1967).

[13] Barnhill, R.E., Optimal quadratures in $L^2(\epsilon_\rho)$II, SIAM J. Numer. Anal., 4, 534-541, (1967).

[14] Barnhill, R.E. and Wixom, J.A., Quadratures with remainders of minimum norm I. Math. Comp., 21, 66-75, (1967).

[15] Barnhill, R.E. and Wixom, J.A., Quadratures with remainders of minimum norm II, Math. Comp., 21, 382-387, (1967).

[16] Barnhill, R.E., Asymptotic properties of minimal norm and optimal quadrature, Numer. Math., 12, 384-393, (1968).

[17] Barnhill, R.E., An error analysis for numerical multiple integration I, Math. Comp., 22, 98-109, (1968).

[18] Barnhill, R.E., An error analysis for numerical multiple integration II, Math. Comp., 22, 286-292, (1968).

[19] Barnhill, R.E. and Nelson, G.M., An error analysis for numerical multiple integration III, Math. Comp., 24, 301-314, (1970).

[20] Barrer, R.B. and Leob, H.L. and Werner, H., On the existence of optimal integration integration formulas for analytic functions, Numer. Math., 23, 105-117, (1974).

[21] Berg, L., Necessary stability conditions for discretization methods concerning boundary value problem of ordinary differential equation, Z. Angew. Math. Mech., 57, 342-344, (1977).

[22] Bergman, S., The kernel functions and conformal mapping. American Mathematical Society, New York, (1950).

[23] Beyn, Wolf-Jurgen, Discrete Green's function and strong stability properties of the finite difference method. Appl. Anal., 14, 73-98, (1982).

[24] Bickart, T.A. and Jury, E.I., Arithmatic tests for A-stability, A[α]-stability and stiff- stability, BIT, Nordisk Tidrkr. Inform.-behandl., 18, 9-21, (1978).

[25] Boutayeb, A. and Twizell, E.H.,Finite difference methods for twelfth-order boundary value problems, Journal of Computational and Applied Mathematics, 35, 133-138, (1991).

[26] Boyce, W.E. and Di Prima,R.C., Elementary differential equation and boundary value problems, John Wiley and Sons, fourth edition.

[27] Brij Bhusan, Optimal multistep methods for first order differential equations in Hilbert spaces of analytic functions, Ph.D. Thesis, Indian Institute of Technology, Kanpur, (1986).

[28] Brown, R.L., Error behavior of multistep methods applied to unstable differential systems. Appl. Math. Modelling, 2, 115-118, (1978).

[29] Brunner, H., Stabilization of optimal difference operators. Z. Angew. Math. Phys., 18, MR 36, 1111, 438-444, (1967).

[30] Butcher, J.C., Linear and non-linear stability for general linear methods, BIT, 27, 182-189, (1987).

[31] Cash, J.R., On the exponential fittings of composite multiderivative linear multistep methods, SIAM J. Numer. Analysis 18, 808-821, (1981).

[32] Cash, J.R. and Singhal, A., High order methods for the numerical solution of two-point boundary value problems, BIT, 22, 184-199, (1982).

[33] Cash, J.R., A variable order deferred correction algorithm for the numerical solution of nonlinear two-point boundary value problem, Comput. Math. Appl., 9, 257-265, (1983).

[34] Chandra, J. and Davis, P.W., A monotone method for quasi linear boundary value problems, Arch. Rational Mech. Anal. 54, 257-266, (1974).

[35] Chawla, M.M. and Riana, B.L., On optimal quadratures for analytic functions, BIT, 12, 489-502, (1972).

[36] Chawla, M.M. and Kaul, V., Optimal rules for numerical integration round the unit circle, BIT, 13, 145-152, (1973).

[37] Chawla, M.M. and Kaul, V., Optimal rules with polynomial precission for Hilbert spaces possessing reproducing kernel functions. Numer. Math., 22, 207-218, (1974).

[38] Chawla, M.M. and Kaul, V., Optimal rules with polynomial precission for Hilbert spaces possessing reproducing kernel functions II, Error bounds, Numer. Math., 25, 379-382, (1976).

[39] Chawla, M.M., An eighth order tridiagonal finite difference method for nonlinear two-point boundary value problems, BIT, 17, 281-285, (1977).

[40] Chawla, M.M., A sixth-order tridiagonal finite difference method for non-linear two point boundary value problems, BIT, 17 128-133, (1977).

[41] Chawla, M.M., High accuracy tridiagonal finite difference approximations for non-linear two-point boundary value problems, Journal of IMA, 22, 203-209, (1978).

[42] Chawla, M.M., A sixth order tridiagonal finite difference method for general two-point boundary value problems with non-linear boundary conditions, Journal of IMA, 24, 35-42, (1979).

[43] Chawla, M.M.and Katti ,C.P.,Finite difference methods for a class of two point boundary value problems with mixed boundary conditions, J. Compu. Appl. Math., 6(3), 189-196, (1980).

[44] Chawla, M.M.and Katti,C.P. ,Finite difference methods and their convergence for a class of singular two point boundary value problems, Numer. Math., 39, 341-350, (1982).

[45] Chawla, M.M. and Katti C.P., A finite difference method for a class of singular two-point boundary value problems, IMA Journal of Numerical Analysis, 4, 457-466, (1984).

[46] Chawla, M.M., On the numerical integration of a singular two point boundary value problems, Intern. J. Computer. Math., 31, 187- 194, (1990).

[47] Chawla, M.M. and Katti, C.P., A uniform mesh finite difference method for a class of singular two point boundary value problems, SIAM J. Numer. Anal., 22, 3, 561-565, (1985).

[48] Chawla ,M.M., McKee, S. and Shaw, G.,Order h^2 method for a class of singular two point boundary value problems, BIT, 26, 318- 326, (1986).

[49] Chawla, M.M., A fourth-order finite difference method based on uniform mesh for a class of singular two point boundary value problems, J. Comp. Appl. Math, 17, 359-364, (1987).

[50] Chawla, M.M. and Kumar, S., Existence uniqueness of the solutions for a class of singular two point boundary value problems. JCAM, 19, 379-388, (1987).

[51] Chen, J., On attainable order of zero -stable linear multistep method in ordinary differential equation, Numer. Math. Nanking, 9, No. 3, 253-257, (1987).

[52] Ciarlet, P.G., Natterer, F. and Verga, R.S., Numerical methods of high-order accuracy for singular non-linear boundary value problems, Numer. Math., 15, 87-99, (1970).

[53] Collatz, L., Functional analysis and numerical mathematics, New York, Academic Press, (1966).

[54] Correas, J.M.,Numerical treatment of initial value problems for ordinary differential equations by linear multistep methods with varying coefficients, Proceedings of second conference on differential equations and their applications I (1979).

[55] Cooper, G.J., The order of convergence of general linear multistep method for ordinary differential equation, SIAM J. Numer. Analysis, 15, 643-661, (1978).

[56] Cronzeix, M. and Lisbona, F.J., The convergence of variable stepsize, variable formula, multistep methods, SIAM J. Numer. Analysis, 21, 512-534, (1984).

[57] Cryer, C.W., A new class of highly-stable methods: A_o-stable methods, BIT, 13, 153-159, (1973).

[58] Dahlquist, Germund G., Convergence and stability in the numerical integration of ordinary differential equation, Math. Scand., 4, 33-53, (1956).

[59] Dahlquist, Germund G., A special stability problem for linear multistep methods, BIT, 3, 27-43, (1963).

[60] Dahlquist, Germund G., Error analysis for a class of methods of stiff non-linear initial value problems, Numerical Analysis, Dundee, Springer Lecture Notes in mathematics, nr.506, 60-74, 1975.

[61] Dahlquist, Germund G., On the relation of G - stability to other stability concepts for linear multistep method, Topics in Numerical Analysis 111, Proc. R. Inst. Acad. Conf., Dublin, 1976, 67-80, (1977).

[62] Dahlquist, Germund G., On one-leg-multistep methods, SIAM J. Numer. Analysis, 20, 1130-1138, (1983).

[63] Dahlquist, Germund G., Liniger, Wernei and Nevanlinna, Olavi, Stability of 2-step methods for variable integration steps, SIAM J. Numer. Analysis, 20, 1071-1085, (1983).

[64] Davis, P.J., Errors of numerical approximation for analytic functions, Survey of Numerical Analysis, John Todd (Ed.) McGraw Hill, New York, 468-484, (1962).

[65] Davis, P.J., Interpolation and approximation, Blaisdell, New York, (1963).

[66] Davis, P.J., Numerical integration, Blaisdell, New York, (1967).

[67] Day, J.D., Codmments on T.D. Bui, On an L-stable method for stiff differential equations, Inf. Process. Lett., 11, 31-32, (1980).

[68] De Branges, L., Hilbert spaces of entire functions, Prentice -Hall, Englewood Cliffs, N.J., MR 37, # 4590, (1968).

[69] De Hoog ,F.R and Weiss,R., Difference methods for boundary value problems with a singularity of the first kind, SIAM J. Numer. Anal, 13,5, 775-813, (1976).

[70] De Hoog, F.R and Weiss,R.,The numerical solution of boundary value problems with an essential singularity, SIAM J. Numer. Anal, 16, 4 ,637-669, (1979).

[71] De Hoog, F.R and Weiss,R., The boundary value problem for systems of ordinary differential equations with singularity of the second kind, SIAM J. Numer, Anal, 11,1, 41-60, (1980).

[72] Dekker, K., Stability of linear multistep method on the imaginary axis, BIT, 21, 66-79, (1981).

[73] Dekker, K., On the order of composite multistep methods for ordinary differential equation, Numer. Math., 29, 381-396, (1978).

[74] Dettman, J.W., Mathematical methods in physics and engineering, McGraw Hill Book Company.

[75] Doedel, E.J., The construction of finite difference approximations to ordinary differential equations, SIAM. J. Numer. Analysis, 15, 450-465, (1978).

[76] Doedel, E.J. and Reddien, G.W., Finite difference methods for singular two point boundary value problems, SIAM J. Numer. Anal., 16, 173-185, (1979).

[77] Doedel, E.J. and Reddien, G.W., Difference methods for singular two point boundary value problems, approximation theory III (Proc. Conf. Univ. Texas, Austin), 349-354, Academic Press, New York, (1980).

[78] Doedel, E.J. and Reddien, G.W., Finite difference methods for singular two point boundary value problems, SIAM J. Numer. Anal., 21, 2, 300-313, (1984).

[79] Eirola, Timo and Nevanlinna, Olavi, What do multistep methods approximate? Numer. Math., 53, No. 5, 559-569, (1988).

[80] Fatunla, Simeon Ola, Nonlinear multistep methods for initial value problem, Comput. Math. Appl., 8, 231-239, (1982).

[81] Fatunla, Simeon Ola, New predictor corrector formulas for initial value problems in ordinary differential equations. Int. J. Comput. Math., 26, No. 3/4, 247-261, (1989).

[82] Finney, P.H. and Price, T.E., Jr., Minimum norm quadratures which satisfy nonstandard interpolating conditions. SIAM J. Numer. Analysis, 23, 210-216, (1986).

[83] Fox, L., Numerical methods for boundary value problems computational techniques for ordinary differential equations, Proc. Conf. Manchester, 175-216, (1980).

[84] Frank, Reinhard, Schneid, Josef and Veberhuber, Christoph W., The concept of B-convergence, SIAM J. Numer. Analysis, 18, 753-780, (1981).

[85] Friedli, A. and Jeltsch, R., An algebraic test for A_o-stability, BIT, Nordisk Tidskr. Inform.-behandl., 18, 402-414, (1978).

[86] Frivali daski Sandor, Predictor corrector methods with variable coefficients, Eotvos Lorand University Computing Centre, Budapest, 61pp, (1983).

[87] Gantschi, W., Numerical integration of ordinary differential equations based on trigonometric polynomials, Numer. Math., 3, 381-397, (1961).

[88] Gear, C.W. and Tu, K.W., The effect of variable mesh size on the stability of multistep methods, SIAM J. Numer. Analysis, 11, 1025-1043, (1974).

[89] Gear, C.W. and Watanable, D.S., Stability and convergence of variable order multistep methods. SIAM J. Numer. Analysis 11, 1044-1058, (1974).

[90] Gear, C.W., Numerical solution of ordinary differential equations: is there any thing left to do? SIAM Review, 23, 10-24, (1981).

[91] Geng, S., Unconditional stable explicit methods, Math. Numer. Sin., 5, 280-294, (1983).

[92] Glushkov, V.M., Psbienichny, B.N. and Bulanyj, A.P., Parallel algorithm for the solution of boundary value problem for systems of differential equations, Cynernetics, 16, 868-872 (1981).

[93] Grigorieff, Rolf D., Stability of multistep methods on variable grids, Numerische Mathematik, 42, 359-377, (1983).

[94] Hairer, E. and Turke, H., The equivalence of B-stability and A-stability, BIT, 24, 520-528, (1984).

[95] Hamming, R.W., Stable predictor- corrector methods for ordinary differential equations, Ibid., 6, 37-47, (1959).

[96] Henrici, P., Discrete variable methods in ordinary differential equations, John Wiley and Sons, Inc. NY, (1962).

[97] Houwen, P.J. van der and Verwer, J.G., Generalized linear multistep methods. I, Development of algorithms with zero-parasitic roots, Math. Centrum, Amsterdam, Afd. Numer. Wirk., NW-10, 16p (1976).

[98] Hull, T.E. and Newbery, A.C.R., Corrector formulas for multistep integration methods, J. Soc. Indust. Appl. Math., 10, MR 27, # 2130, 351-369, (1962).

[99] Iserles, A., Nonlinear stability and asymptotics of ordinary differential equation solvers, Numerical mathematics. Proc. Int. Conf. Singapore 1988, ISNM, Int. Ser. Numer. Math., 86, 225-236, (1988).

[100] Jain, M.K., Numerical solutions of ordinary differential equations, Wiley Eastern, New Delhi, (1984).

[101] Jain, R.K. and Jain, P., Finite difference methods for a class of singular two-point boundary value problems, Intern. J. Comp. Math., 27, 113-120, (1989).

[102] Jeltsch, R., Stiff stability and its relation to A_o and A(O) stability, SIAM J. Numer. Analysis, 13, 8-17, (1976).

[103] Jeltsch, R., Note on A-stability of multistep multiderivative method, BIT Nordisk Tidskr. Inform-behandl., 16, 74-78, (1976).

[104] Jeltsch, R., A necessary condition for A-stability of multistep multiderivative methods, Math. Comput., 30, 739-746, (1976).

[105] Jeltsch, R., Stiff stability of multistep multiderivative methods, SIAM J. Numer. Analysis, 14, 760-772, (1977).

[106] Jeltsch, R., On generalized linear multistep method with zero-parasitic roots of an adaptive principal root, Numerische Math., 27, 143-155, (1977).

[107] Jeltsch, R., Stability on the imaginary axis and a stability of linear multistep method, BIT, Nordisk. Tidskr. Inform.-Behandl., 18, 170-174, (1978).

[108] Jeltsch, R., A_o-stability and stiff stability of Brown's multistep multiderivative methods. Numerische Math., 32, 167-181, (1979).

[109] Jeltsch, R., Corrigendum: Stiff stability of multistep multiderivative methods, SIAM J. Numer. Analysis, 16, 339-345, (1979).

[110] Jeltsch, R. and Nevanlinna, O., Stability of explicit time discretizations for solving initial value problem, Numer. Math., 37, 61-91, (1981).

[111] Katti, C.P and Chopra, K., On the stability of modified numerov method for solving a class of singular two point boundary value problems, International Journal of Comuter Mathematics, Vol. 37, 221-226, (1990).

[112] Kaul, V., Optimal rules for the numerical integration of periodic analytic functions. Notices of Amer. Math. Society, 74 T-C31, 31, A 498, (1974).

[113] Kaul, V., Optimal approximation in Hilbert spaces possessing reproducing kernel functions, Ph.D. Thesis, Indian Institute of Technology, New Delhi, (1974).

[114] Kedem, G., A posteriori error bounds for 2-point boundary value problem, SIAM J. Numer. Analysis, 18, 431-448, (1981).

[115] Keller, Herbert B., Numerical methods for two point boundary value problems, Blaisdell Publishing Company, Massachusetts, (1968).

[116] Koloza, J., Stability of the 2nd derivative linear multistep formulas, Acta Univ. Palack. Olomuc. Fac. Rer. Natur., 53, Math. 16, 167-184, (1977).

[117] Koloza, J., A necessary condition for B-stability, BIT, Nordisk. Tidskr. Inform.-behandl., 19, 111-115, (1979).

[118] Kraaijevanger, J.F.B.M., B-convergence of the implicit midpoint rule and the trapezoidal rule, BIT, 25, 652-666, (1985).

[119] Krasnosel'skii, M.A. and Stecenko,V.J., Some non-linear problems with matrix solutions, Sibirsk. Mat. Z. 4, 29-48, (1963).

[120] Kirchgraber, U., Multistep methods are essentially one-step methods, Numer. Math., 48, 85-90, (1986).

[121] Lambert, J.D., Linear multistep method with mildly varying coefficients, Math. Comput., 24, 81-93, (1970).

[122] Lambert, J.D. and Shaw, B., A method for numerical solution of y' = f(x,y) based on self adjusting non-polynomial interpolant, Math. Comp., 20, 11-20, (1966).

[123] Lambert, John D. and Shaw, Brian, A generalization of multistep methods for ordinary differential equation, Numerische Math., 8, 250-263, (1966).

[124] Lambert, J.D. and Sigurdsson, S.T., Multistep methods with variable matrix coefficients, SIAM J. Numer. Analysis, 9, 715-733, (1972).

[125] Lapidus, L. and Seinfeld, J.H., Numerical solution of ordinary differential equations. Academic Press, New York, (1971).

[126] Larkin, F.M., Optimal approximation in Hilbert spaces with reproducing kernel functions, Math. Comp., 24, 911-921, (1970).

[127] Lees, M., Discrete methods for nonlinear two-point boundary value problems, Numerical solution of partial differential equations (Bramble, J.H., Ed.), New York, Academic Press, 59-72, (1966).

[128] Li, Shoufu, The measure of stability of discrete variable methods, Nat. Sci. J. Xiangtan Univ., No. 2, 47-62, (1984).

[129] Li, Wangyaa, Asymptotically A-stable linear K-step methods. Sci. Sin. Ser. A, 26, 251-258, (1983).

[130] Liniger, W., A criterion for A-stability of linear multistep integration formulae, Computing, 3, 280-285, (1968).

[131] Liniger, W., Connections between accuracy and stability properties of linear multistep formulas, Commun. ACM, 18, 53-56, (1975).

[132] Marz, R., Variable multistep methods, Prepr. Neue Folge, Humboldt Univ., Berlin, Sekl. Math., 7, 31p, (1981).

[133] Marz, R., On the stability of variable methods in initial value problem and in boundary value problem, Seminarber, Humboldt Univ., Berlin Sekt. Math., 32, 43-63, (1981).

[134] Marz, R., Variable multistep methods, Computational Mathematics, Banach Cent. Publ., 13, 407-424, (1984).

[135] Maurce O' R., Exponential fitting applied to quasi -linear two point boundary value problem BAIL IV, 387-391, Boole Press Conf. Ser. 8, Boole Dim Laoghire, (1986).

[136] Mckee, Pitcher, N., On the convergence of advanced linear multistep method, BIT, Nord. Tidskr., Inform-behandl, 19, 476-481, (1979).

[137] Mihelcic, M., $A(\alpha)$-stable cyclic composite multistep methods of order 5, Computing, 20, 267-272, (1978).

[138] Mihelcic, M. and Wigerath, K., $A(\alpha)$-stable cyclic composite multistep methods of orders 6 and 7 for numerical integration of stiff ordinary differential equation, Z. Angew. Math. Mech., 61, 261-264, (1981).

[139] Natterer, F., A generalized spline method for singular boundary value problems of ordinary differential equations, Linear Algebra and Appl., 7, 189-216, (1973).

[140] Neta, B. and Ford, C.H., Families of methods for ordinary differential equations based on trigonometric polynomials, J. Comput. Appl. Math., 10, 33-38, (1984).

[141] Ng, B.S. and Reid, W.H., A numerical method for linear 2-point boundary value problem using compound matrices, J. Comput. Phys., 33, 70-85, (1979).

[142] Niznik, Carol A., A numerical analysis of 2-point boundary value problem algorithm, J. Comput. Appl. Math., 6, 201-211, (1980).

[143] Norsett, S.P., A criterion for $A(\alpha)$ stability of linear multistep method BIT, Vol. 9, 259-263, (1969).

[144] Odeh, F., Some stability techniques for multistep methods, IBM J. Res. Dev., 31, 178-186, (1987).

[145] Odeh, F. and Liniger, W., Nonlinear fixed-h stability of linear multistep formulas, J. Math. Analysis Appl., 61, 691-712, (1977).

[146] Oliwer, P., A family of linear multistep method for the solution of stiff and nonstiff ordinary differential equation, IMA J. Numer. Anal., 2, 289-301, (1982).

[147] Oliveira, P. and Patricio, F., Instability in linear multistep method, Appl. Analy., 28, No. 1, 1-14, (1988).

[148] Onumanyi, P. and Ortiz, E.L., Numerical solution of high order boundary value problem for ordinary differential equation with an estimations of the error, Int. J. Numer. Methods Eng., 18, 775-781, (1982).

[149] Pandey, R.K., A study of some singular two point boundary value problems, Ph.D. Thesis, Indian Institute of Technology, Kanpur, (1991)

[150] Pinkus, A., Asymptotic minimum norm quadrature formula, Numer. Math., 24, 163-175, (1975).

[151] Rabinowitz, P. and Ritcher, N., Asymptotic properties of minimal integration rules, Math. Comp., 24, 593-609, (1970).

[152] Rabinowitz, P. and Ritcher, N., Chebyshev type integration rules of minimum norm, Math. Comp., 24, 831-845, (1970).

[153] Ralston, A., Relative stability in the numerical solution of ordinary differential equations, SIAM Rev., 7, 114-125, (1965).

[154] Ralston, A. and Rabinowitz, P., A first course in numerical analysis, McGraw Hill, (1978).

[155] Rathore, R.K.S., Linear algebra and applied matrix theory, Manuscript, Indian Institute of Technology, Kanpur, (1994).

[156] Rentrop ,P., A Taylor series method for the numerical solution of two point boundary value problems, Numer. Math., 31 359-375, (1979).

[157] Richter, N., Properties of minimal integration rules, SIAM J. Numer. Analysis, 7, 67-79, (1970).

[158] Richter, N., Properties of minimal integration rules II, SIAM J. Numer. Analysis, 8, 497-508, (1971).

[159] Richter, N., Minimal interpolation and approximation in Hilbert spaces, SIAM J. Numer. Anal., 8, 583-597, (1971).

[160] Rockwold, Gary K., A_o-stable linear multistep formulas of the α-type, BIT, 27, 123-128, (1987).

[161] Rose, M.E., Finite difference schemes for differential equations, Math. Comp. 18, 179-195, (1964).

[162] Royden, H.L., Real analysis, Macmillan Publishing Company, New York, (1963).

[163] Rudin, W., Real and complex analysis, McGraw-Hill Book Company, New York (1974).

[164] Sanz-Serna, J.M., Linearly-implicit variable coefficient methods of Lambert-Sigurdsson type, IMA J. Numer. Analysis, 1, 39-46, (1981).

[165] Sard, A., Best approximate integration formulas. Amer. J. Math., 71, 80-91, (1949).

[166] Scraton, R.E., Some L-stable methods for stiff differential equations, Int. J. Comput. Math., 9, 81-87, (1981).

[167] Setter, H.J., Analysis of Discretization for Ordinary Differential Equations, Springer Verlag, Berlın, Heidelberg, New York, (1973).

[168] Shampine, L.F., Boundary value problems for ordinary differential equations, SIAM J. Numer. Anal.,5 ,2, 219-242, (1968).

[169] Shampine, L.F., Boundary value problems for ordinary differential equations. II : Patch bases and monotone methods, SIAM J. Numer. Anal. 6, 3, 414-431, (1969).

[170] Shampine, L.F. and Gordon,M.K., Computer solutions of ordinary differential equations : The initial value problem, W.H. Freeman,San Francisco, (1975).

[171] Shaw, B., Modified multistep methods based on a nonpolynomial interpolant, J. Assoc. Comput. Machin., 14, 143-154, (1967).

[172] Sigurdsson, S., Linear multistep methods with variable matrix coefficients, Conf. Appl. Numerical Analysis, Dundee, Lecturenotes Math., 228, 327-331, (1971).

[173] Skeel, Robert D. and Kong, Antony K., Blended linear multistep methods. ACM Trans. Math. Software, 3, 326-345, (1977).

[174] Skeel, Robert D. and Vu, Thu V., Note on blended linear multistep formulas, ACM Trans. Math. Software, 12, 223-224, (1984).

[175] Spreuer, H., A method for the computation of bounds with convergence of arbitrary order for ordinary linear boundary value problem, J. Math. Anal. Appl., 81, 99-133, (1981).

[176] Steller, Hans J., Analysis of discretization methods for ordinary differential equations, Springer Varlung, Berlin, Heidelberg, New York, (1973).

[177] Szego, G., Orthogonal polynomials, American Mathematical Society, New York, (1939).

[178] Tenenebaum, M. and Pollard, H., Ordinary differential equations , Harper and Row Publisher, New York.

[179] Tewarson ,R.P., A numerical method for solving two point boundary value problems for non-linear ordinary differential equations, Internation Journal for Numerical Methods in Engineering, 464-469, (1980).

[180] Tewarson, R.P., A seventh-order numerical method for solving boundary value non-linear ordinary differential equations, International Journal for Numerical Methods in Engineering, 18, 1313-1319, (1982).

[181] Tewarson, R.P. and Gupta, S., Improving the accuracy of finite difference methods for solving boundary value ordinary differential equations, BIT, 22, 353-360, (1982).

[182] Tewarson ,R.P. and Zhang ,Vin,Solution two-point boundary value problems using splines, International Journal for Numerical Methods in Engineering, 23, 707-710, (1986).

[183] Ticher, P. Sacks-Davis, A new class of cyclic multistep formulae for stiff systems, SIAM J. Sci. Stat. Comput., 4, 733-747, (1983).

[184] Twizell ,E.H.,Numerical methods for sixth-order boundary value problems, International Series of Numerical Mathematics, 86(c), 495-506, (1988).

[185] Twizell ,E.H.and Boutayeb ,A.,Numerical methods for the solution of special and general sixth-order boundary value problems with application to Bernard layer eigenvalue problems, Proceedings of Royal Society London, 431(A), 433-450, (1990).

[186] Van Selow, Reiner, Nonlinear stability behaviour of linear multistep method, BIT, 23, 388-296, (1983).

[187] Varah, J.M., Stiffly stable linear multistep method of extended order, SIAM J. Numer. Analysis, 15, 1234-1246, (1978).

[188] Varga, R.S., Matrix Iterative Analysis, Prentice Hall, Inc., Englewood cliffs, New Jersey, (1962).

[189] Varil'kov, G.D. and Zagonov, V.P., The accuracy of a method for the numerical solution of ordinary differential equation with variable coefficients, Differ. Equations, 19, 843-850, (1983).

[190] Veldhuizen, M. van, D-stability, SIAM J. Numer. Analysis, 18, 45-64, (1981).

[191] Verwer, J.G., Generalized linear multistep methods II: Numerical applications, Math. Centrum, Amsterdam, Afd. Numer. Wisk, NW-12, 35p, (1974).

[192] Verwer, J.G., On generalized linear multistep method with zero-parasitic roots and an adaptive principal root. Numerisch. Math., 27, 143-155, (1977).

[193] Wanner, G., Hairer, E. and Nørsett, S.P., Order stars and stability theorems, BIT, 18, 475-489, (1978).

[194] Wanner, G., A-stability of one and multistep methods, Numerical Ordinary Differential Equations, 1979, Signum Meet, Champaign, Ill., Exp. No. 5, 1-3, (1979).

[195] Wanner, G., Hairer, E. and Nørsett, S.P., When I-stability implies A-stability, BIT, Nordisk. Tidskr., Inform-behandl, 18, 503, (1978).

[196] Widlund, Olof B., A note on unconditionally stable linear multistep method, BIT, 7, 65-70, (1967).

[197] Zlatev, Z., Stability properties of variable stepsize variable formula methods, Numerische Math., 31, 175-182, (1978).

[198] Zlatev, Z., Zero-stability properties of the 3-ordinate variable stepsize variable formula methods, Numer. Math., 37, 157-166, (1981).

[199] Zlatev, Z., Consistency and convergence of general linear multistep variable stepsize variable formula methods, Computing, 31, 47-67, (1983).

[200] Zlatev, Zahari, Variable stepsize variable formula methods based on predictor-corrector schemes, Appl. Numer. Math., 1, 395-416, (1985).